Compilation of chemical indicators

DEVELOPMENT, REVISION , AND ADDITIONAL ANALYSES

2016 edition

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1 Introduction

Eurostat, the statistical office of the European Union, is maintaining indicators on chemicals. Several Member States Competent Authorities and National Statistical Institutes have expressed interest in knowing more about the methodology used to calculate the indicators, with the aim to produce indicators on chemicals management at national level.

This paper provides background information on chemical indicators that are produced by Eurostat([1]):

- 'Production of toxic chemicals'([2]), that is based on chemicals classified for their human health hazards,
- 'Production of environmentally harmful chemicals', that is based on chemicals classified for their environmental hazards, and
- Two related indicators on consumption (i.e. one for human health and one for environmental endpoints).

The first two indicators are based on official statistics on the production of industrial chemicals, compiled by National Statistical Institutes and Eurostat. Production volumes are weighted according to the toxicity of the chemicals (both for human health and environmental endpoints). By adding data from official foreign trade statistics the production-related indicators are expanded to two additional indicators presenting the consumption.

During the past years two major changes have been introduced that have an impact on the methodology of the chemicals indicator system:

- The description of toxic and environmentally harmful characteristics according to the 'old' risk phrases ('R-phrases' hereafter) of the Dangerous Substances Directive([3]) was changed to the hazard statements ('H-statements' hereafter) according to the CLP Regulation([4]), also taking into account self-classifications under REACH (see chapter 5).
- Following the accession of Croatia to the European Union the scope of the indicator is expanded from EU-27 to EU-28. Eurostat's Production Statistics Team operating the PRODCOM database, the project manager and the consultant agreed to use the introduction of the new classification scheme as an opportunity to include statistics from Croatia and to change the coverage from EU-27 to EU-28. The EU-27 indicator will not be published anymore (see discussion in chapter 3).

([1]) The indicators are accessible at Eurostat website: http://ec.europa.eu/eurostat/statistics-explained/index.php/Chemicals_production_statistics.

([2]) This indicator was part of the EU sustainable development indicator (SDI) set used to monitor the EU Sustainable Development Strategy until 2015 and is currently being considered for the EU indicator set on the sustainable development goals.

([3]) Council Directive 67/548/EEC of 27 June 1967 on the approximation of laws, regulations and administrative provisions relating to the classification, packaging and labelling of dangerous substances.

([4]) Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006.

As these major changes and the corresponding updates of the indicators may lead to some confusion of users, this paper discusses both the old and the new version of the indicator system, but also contains additional background information and analyses.

The indicators provide reliable information since they are based on official statistics. They can serve as an independent monitoring instrument and may e.g. be used in the up-coming efficiency assessment of chemical legislation in the European Union.

The paper is divided into the following chapters:

Chapter 2 briefly introduces the principles of the indicators.

Chapter 3 summarises the overall changes in methodology and discusses why and how the changes are implemented.

Chapter 4 provides a summary of the methodology of the 'old' indicator weighting scheme, so the reader is informed about the history of the indicator.

Chapter 5 explains the revisions, e.g. the 'new' indicator weighting scheme according to the CLP Regulation, and includes background information on data retrieval and evaluation.

Chapter 6 shows the latest published versions of both, the 'old' indicator according to R-phrases and the 'new' indicator according to the H-statements of the CLP Regulation.

Finally, Annex 3 provides detailed analyses in relation to the relevance of the indicators, which have no impact on the calculation indicators themselves.

2 Compilation approach of the indicators

Eurostat has developed indicators for the production of toxic chemicals and the production of environmentally harmful chemicals. Both are based on the same approach and use Eurostat production statistics (PRODCOM).

PRODCOM provides statistics on the production of manufactured goods. The term comes from the French 'PRODuction COMmunautaire' (Community Production) for mining, quarrying and manufacturing: sections B and C of the Statistical Classification of Economy Activity in the European Union (NACE Rev. 2).

PRODCOM uses the product codes specified on the PRODCOM List, which contains about 3 900 different types of manufactured products.

- Products are identified by an 8-digit code:
  - the first four digits are the classification of the producing enterprise given by the Statistical Classification of Economic Activities in the European Community (NACE) and the first six correspond to the CPA (Classification of Products by Activity)
  - the remaining digits specify the product in more detail
- Most product codes correspond to one or more Combined Nomenclature (CN) codes, but some (mostly industrial services) do not.

PRODCOM excludes items that are not considered manufactured products (e.g. some agricultural products where the processing is not considered as manufacturing). In the context of these indicators, it is also important to emphasize that PRODCOM does not cover fuel products.

The following categories from PRODCOM are evaluated for the indicators, representing the main categories of chemical production (Table 1). The indicator covers the part of the chemical production that is defined by the NACE codes for the economic sector. The NACE nomenclature has been revised for 2008, leading to a major break in series.

Table 1: PRODCOM categories in NACE Rev.1 and NACE Rev.2

Coverage	NACE Rev.1 (1995-2007)	NACE Rev.2 (2008-)
Manufacture of industrial gases	24.11	20.11
Manufacture of dyes and pigments	24.12	20.12
Manufacture of other inorganic basic chemicals	24.13	20.13
Manufacture of other organic basic chemicals	24.14	20.14
Manufacture of fertilizers and nitrogen compounds	24.15	20.15

These five categories are further divided and contain individual substances or group entries, the highest level of detail is represented by an 8-digit code. For example, PRODCOM code 20.14.11.30 refers to 'ethylene' and PRODCOM code 20.13.24.60 refers to 'oxides of boron; boric acids; inorganic acids (excluding hydrogen fluoride)'.

In a first step, some PRODCOM entries were excluded from the evaluation. For example, some gases (such as hydrogen, nitrogen, oxygen) were not included due to dramatic changes that cannot be explained properly. Note, however, that none of these substances were classified as toxic. For each PRODCOM entry at the 8-digit level the tonnage produced can be retrieved.

In a second step, the hazard information for each PRODCOM entry is retrieved. Until the adoption of the CLP Regulation, the hazard information was based on risk phrases according to the Dangerous Substances Directive([5]), while it is now based on H-statements according to the CLP Regulation([6]). Such an evaluation is straightforward if the PRODCOM entry refers to an individual substance (e.g. ethylene), but is more complicated if the PRODCOM entry relates to a group of substances (e.g. oxides of boron; boric acids; inorganic acids, excluding hydrogen fluoride). In these latter cases, a representative substance for the group was selected early in the process and the hazard information for this substance is retrieved.

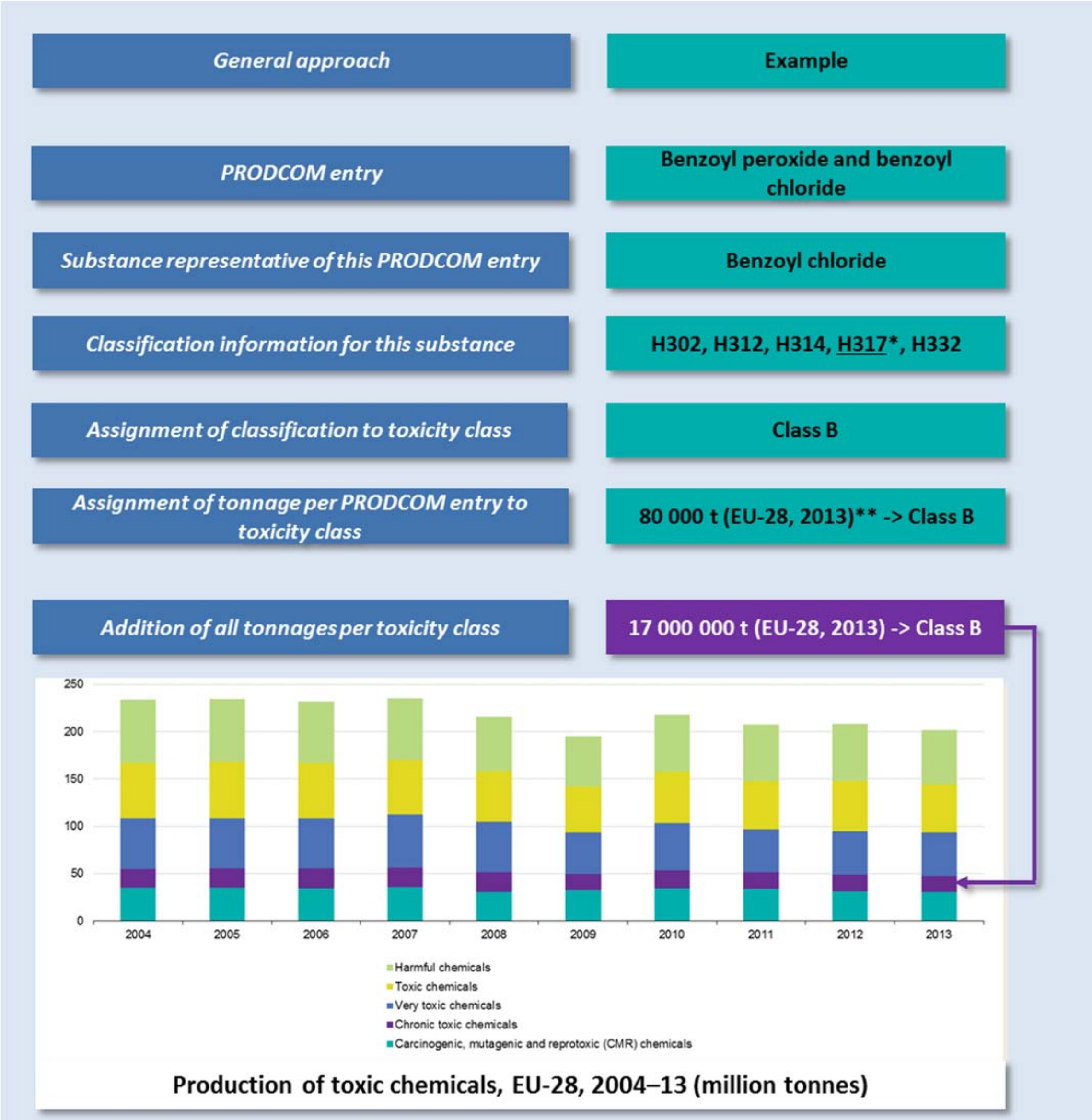
With the tonnage produced and the hazard information available for each PRODCOM entry, the tonnage is aggregated for entries sharing a particular toxic property. For example, it is possible to sum up all tonnages for PRODCOM entries representing substances that are carcinogenic. However, an aggregation based on single toxic properties would become confusing due to the large number of different H-statements. Therefore, an aggregation into five classes (classes A-E) was chosen (e.g. class B: 'chronic toxic chemicals' and class C: 'very toxic chemicals'). The principal approach is shown in the following figure using the example of the PRODCOM entry 'Benzoyl peroxide and benzoyl chloride'([7]). Chapters 4 and 5 provide more details on the assignment to toxicity classes.

([5]) Council Directive 67/548/EEC of 27 June 1967 on the approximation of laws, regulations and administrative provisions relating to the classification, packaging and labelling of dangerous substances.

([6]) Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006.

([7]) Benzoyl chloride was assigned as the reference substance when the indicator was developed, i.e. before REACH entered into force. The REACH registration tonnages support this assignment. The tonnage band for benzoyl chloride is 10-times higher than the one for benzoyl peroxide, illustrating that benzoyl chloride is in fact the better representative for this PRODCOM entry. Both substances are classified for skin sensitisation, resulting in an assignment to class B (see Chapter 5).

Figure 1: Compilation approach for the indicator ‘Production of toxic chemicals’



* H-statement leading to the highest toxicity class
** Non-confidential PRODCOM tonnage for ‚Benzoyl peroxide and benzoyl chloride’ shown here for illustrative purposes. In the indicator calculation, the confidential PRODCOM tonnage is used.

This paper focusses on the indicator ‘Production of toxic chemicals’, the approach taken for the compilation of the other indicators is similar to this indicator.

3 Changes in the toxic chemicals indicator

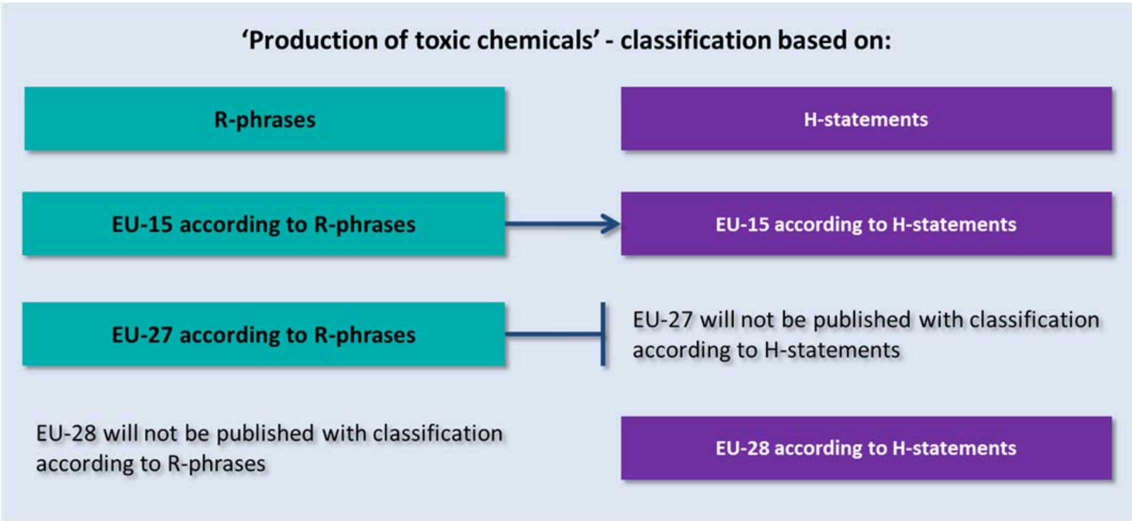
The indicator on the 'Production of toxic chemicals' has undergone two fundamental changes in recent years.

The first one, the change from the R-phrases (based on the Dangerous Substances Directive) to the H-statements according to the CLP Regulation, was also used to re-engineer the older classification scheme and to include additional information from registration dossiers submitted under REACH (see chapter 5).

The second major change had to be made after the accession of Croatia as the 28th Member State of the EU: Confidentiality problems with the production statistics would arise if EU-27 and EU-28 were published together. Differences in indicator values could in this case be attributed to Croatia and may (today or in the future) disclose confidential data.

However, as the PRODCOM data for Croatia is available from 2004 onwards, the publication of an EU-28 indicator is possible if a new aggregation scheme is introduced at the same time. The new aggregation scheme according to H-statements allows publishing the data without any confidentiality conflicts. The approach taken to ensure confidentiality is shown in Figure 2.

Figure 2: Development of the revised indicator 'Production of toxic chemicals'



The new set of indicators is therefore:

1. The EU-15([8]) indicator on toxic chemicals according to the CLP aggregation scheme from 1996([9])-2014 and beyond. Although this indicator deals only with 15 Member States it covers the largest part of the EU chemical industry (about 80 %) and has the longest time series, allowing for tracking changes in the chemical production for 2 decades (in 2015),
2. The EU-28 indicator on toxic chemicals according to the CLP aggregation scheme from 2004-2014 and beyond. This indicator captures the entire European Union.

The indicators based on the ‘old’ aggregation according to the R-phrases will not be published anymore. The EU-27 indicator on the consumption of toxic chemicals according to R-phrases will be exchanged with the EU-28 indicator with an aggregation based on H-statements.

([8]) EU-15 was the number of member countries in the European Union prior to the accession of ten candidate countries on 1 May 2004. The EU15 comprised the following 15 countries: Austria, Belgium, Denmark, Finland, France, Germany, Greece, Ireland, Italy, Luxembourg, the Netherlands, Portugal, Spain, Sweden and the United Kingdom.

([9]) Eurostat’s PRODCOM statistics started in 1995. However, the data for the first year show a significant amount of data gaps.

4 Toxic chemicals: aggregation scheme according to R-phrases and changes in the PRODCOM database

4.1. Introduction

The ‘old’ indicator ‘Production of toxic chemicals’ sums up the production volumes of chemicals classified for human health hazards. Eurostat’s PRODCOM database, a statistical database that provides production data of the Member States, serves as the basis. The PRODCOM database contains the total production of the covered industry in volumes manufactured, as well as in monetary values within the statistical coverage (threshold due to size of manufacturers, etc.). Only if the PRODCOM entries are detailed enough, e.g. if the product covers a single process or a well-defined product, we are able to identify a ‘chemical’ to which attributes concerning physical, chemical or toxic properties could be added. Fortunately, the statistics focus on major chemicals with a high production value and volume. As long as the indicator derived from this database is based on volume the result is estimated to be fairly correct. The products in PRODCOM which cannot be attributed to a ‘toxic chemicals class’ may also contain toxic chemicals. Therefore, these products should not be called ‘non-toxic, they are referred to as ‘non-toxic and others’ in the evaluations below.

4.2. Classification of chemicals by toxicity class

The chemicals are assigned to five aggregated classes according to their specific toxicity as shown in Table 2. The classes represent the hazard of a chemical, but allow no judgement on exposure and risk.

Table 2: Classification of toxic properties

Class	Description
A	CMR chemicals: carcinogenic, mutagenic and reproductive toxicants
B	Suspected to be carcinogenic, mutagenic and reproductive toxicants as well as skin and respiratory sensitizers (collectively called chronic toxic chemicals)
C	Very toxic chemicals
D	Toxic chemicals
E	Harmful chemicals

The classification uses the R-phrases, as obtained e.g. from safety data sheets, with the aggregation shown in Table 3. Class A and B primarily describe chronic toxicity. Class A consists of chemicals with carcinogenic or mutagenic properties as well as reproductive toxicants (CMR substances). Suspected CMR chemicals form class B, together with sensitising substances. Class C, D and E describe acute toxic effects as ‘very toxic’ (C), ‘toxic’ (D) and ‘harmful’ (E).

Table 3: Classification by R-phrases

Class	Risk phrases							
A	R45	R46	R49	R60	R61			
B	R42	R43	R64	R40	R62	R63		
C	R26	R27	R28	R32	R48/23	R48/24	R48/25	R35
D	R23	R24	R25	R34	R29	R31		
	R33	R41	R48/20	R48/21	R48/22			
E	R20	R21	R22	R65	R36	R37	R38	

Every chemical produced in the sectors (NACE classes) 20.11. to 20.15., which can be classified by an R-phrase, is aggregated to the corresponding toxicity class. Chemicals, which can be characterised by more than one R-phrase, are characterised by the highest ranked R-phrase starting from class A to E. This system allows building five classes without needing any additional expert ranking. The different classes (A-E) are then shown in mass units.

4.3. Changes in the PRODCOM database

Due to several revisions in the PRODCOM database, the coverage of the indicator (R-phrase and CLP alike) as shown in Table 1 above has changed.

Whilst these revisions are at first a rearrangement of economic sectors that leaves statistics for the single product intact, the steady on-going internal revisions have taken a toll on the number of chemicals covered by the indicator.

Table 4: Coverage of chemicals and identified toxic chemicals

Year	Number of PRODCOM entries representing chemicals	Number of PRODCOM entries representing toxic chemicals
1995	393	170
1996-2001	391	170
2002	389	166
2003-2006	383	165
2007	374	158
2008	306	110 + 20*

* Products with ‘mixed’ classifications; see text below for details.

As shown in the table above, the number of PRODCOM entries has declined over time, especially after the 2008 revision. Please note that the overall coverage (in economic terms or total volume) has not been reduced. Products representing chemicals that are not produced anymore have been deleted and products with small volume have been aggregated.

Until 2007, this aggregation does not affect the indicators. If aggregated, the new aggregated products include older products of the same toxicity classification. In contrast, the 2008 revision strongly affects the establishment of the indicator as positions have been aggregated. As an example, the products

24.14.73.20 *Benzene* (class A – CMR) and

24.14.73.30 *Toluene and xylenes* (class E – harmful)

have been aggregated to: 20.14.73.20 *Benzene, toluene and xylenes*.

In this case, products have been aggregated, which include chemicals that are classified differently (as shown above). To overcome this problem an internal allocation procedure is performed. The current volume of the new product is distributed to the classes according to the 2007 share of the 'old' products. For chemicals with smaller volumes this procedure might be reasonable, but for chemicals with higher volumes the indicator becomes less robust. Nonetheless, this approach is favoured over elimination of these products from the indicator.

This procedure affects 20 products with 'mixed' classifications for toxic chemicals. For 2008, a detailed review shows that the coverage for the NACE Rev. 2 is equivalent to the NACE Rev. 1. From then on, this approach might introduce uncertainty as it relies on 2007 data.

5 Revision of the indicators

5.1. Revision of hazard information: replacement of risk phrases by hazard statements

5.1.1. Background

As summarised in chapters 2–4, the indicators on production and consumption were previously based on risk phrases (‘R-phrases’). One of the main changes introduced by the CLP Regulation of 2008 relates to the description of hazardous properties of substances. The CLP Regulation describes hazardous properties by hazard statements (‘H-statements’) that replace the risk phrases.

As a consequence, the methodology of the production and consumption indicators had to be adapted to the new system of H statements. While a straightforward translation of R-phrases to H statements and the subsequent assignment of an indicator class would have been feasible in some cases, a complete revision of the hazard classification for all substances covered by the indicators was considered more meaningful, because:

- the R-phrases of self-classifications (see below) previously had to be collected from different sources and required an update and
- ECHA’s Classification and Labelling (C & L) Inventory became available that allowed central access to all relevant classification information.

The CLP Regulation requires manufacturers and importers placing a chemical on the market to notify the classification and labelling information to the European Chemicals Agency (ECHA). The Agency in turn is required under Article 42 of the CLP Regulation to establish and maintain a Classification and Labelling Inventory (C & L Inventory) and to make this information publicly available. ECHA fulfilled its obligation with the publication of the C & L Inventory in February 2012. The Inventory is updated regularly.

The information contained in the Classification and Labelling Inventory is considered an important source and the following paragraphs describe a methodology for using these data for the revision of the hazard data used in the indicator system.

5.1.2. Content of the Classification and labelling Inventory

The Inventory not only contains the harmonised classification according to Annex VI([10]) of the CLP Regulation, but millions of self-classification entries, together reflecting classification and labelling information for about 100 000 substances([11]). While thus providing important hazard information for several thousand substances without a harmonised classification, it must be stressed that the C & L Inventory data (i.e. the non-harmonised data from self-classifications) have not been checked by ECHA as to their validity and reliability. As a consequence, some classification and labelling information for the same substance appear to be confusing (see below). However, there may also be justifications for diverging classifications. For example, the same substance may have different impurity profiles (not made public in the C & L Inventory for confidentiality reasons), resulting in a different classification.

As an example for confusing classification information, the entries for *lithium hydroxide* (CAS([12]) number 1310-65-2; information retrieved in August 2014) are shown in Figure 3.

([10]) Annex VI lists hazardous substances for which harmonised classification and labelling have been established at European Union level.

([11]) ECHA Newsletter, No. 2, April 2012.

([12]) CAS: Chemical Abstract Service

Figure 3: Screenshot of information from the C & L Inventory for lithium hydroxide*

Classification		Labelling			Specific Concentration limits, M-Factors	Notes	Classification affected by Impurities / Additives	Additional Notified Information	Number of Notifiers	Joint Entries	View
Hazard Class and Category Code(s)	Hazard Statement Code(s)	Hazard Statement Code(s)	Supplementary Hazard Statement Code(s)	Pictograms, Signal Word Code(s)							
Met. Corr. 1	H290	H290		GHS05 Dgr					437		
Skin Corr. 1C	H314	H314									
Eye Dam. 1	H318	H318									
Aquatic Chronic 3	H412	H412									
Skin Corr. 1A	H314	H314		GHS05 Dgr				State/Form IUPAC Names	93		
Eye Dam. 1	H318	H318									
Aquatic Chronic 3	H412	H412									
								State/Form	65		
Not Classified									39		
Acute Tox. 3	H301	H301		GHS06 GHS05 Dgr				State/Form IUPAC Names	28		
Skin Corr. 1A	H314	H314									
Acute Tox. 3	H331	H331									
Acute Tox. 4	H302	H302		GHS05 Dgr				State/Form IUPAC Names	19		
Skin Corr. 1A	H314	H314									
Acute Tox. 4	H302	H302		GHS07 GHS09 GHS05 Dgr				State/Form Additional CAS Numbers IUPAC Names	19		
Skin Corr. 1B	H314	H314									
Aquatic Chronic 2	H411	H411									
Skin Corr. 1A	H314	H314		GHS05 Dgr				IUPAC Names	18		
Eye Dam. 1	H318										
Acute Tox. 4	H302	H302		GHS07 GHS05 Dgr				State/Form IUPAC Names	18		
Skin Corr. 1B	H314	H314									
Aquatic Chronic 3	H412	H412									
Acute Tox. 4	H302	H302		GHS07 GHS05 Dgr				State/Form Additional CAS Numbers IUPAC Names	16		
Skin Corr. 1A	H314	H314									
Acute Tox. 4	H302	H302		GHS07 GHS05 Dgr	M(Chronic)=0			State/Form IUPAC Names	10	✔	
Skin Corr. 1B	H314	H314									
Skin Corr. 1A	H314	H314		GHS05 Dgr				State/Form IUPAC Names	7		
Acute Tox. 4	H302	H302		GHS07 GHS05 Dgr				State/Form IUPAC Names	4		
Skin Corr. 1A	H314										
		H312									
Acute Tox. 3	H301	H301		GHS06 GHS05 Dgr				State/Form IUPAC Names	4		
Skin Corr. 1A	H314	H314									

* The main information discussed below is in the first two columns ('Classification'). Diverging classifications are identified by alternating shades of the rows and the corresponding number of notifiers.

Many different self-classifications exist for the substance, which are hierarchically ordered by the number of notifiers (only the top entries are shown here) but there is no harmonised classification. The example shows in relation to human health and environmental hazards the following:

- While most notifiers considered the substance to be corrosive to skin ('skin corr.' in column 1), there was disagreement about the potency with categories 1A, 1B and 1C assigned by the notifiers.
- Some notifiers assigned both H318 ('causes serious eye damage') and H314 ('causes severe skin burns and eye damage'). According to the respective Guidance (ECHA, 2012c), this is not indicated since H314 already covers H318 (see wording above).
- An acute toxicity (human health) classification has only been assigned by comparatively few notifiers and these differ somewhat (Acute Tox. 3 and 4, respectively).
- The substance is classified by many, though not all, notifiers for aquatic chronic toxicity, with some differences observed (category 2 and 3), respectively.

The reason for these different classifications is unclear. However, several possible explanations exist. For example, skin corrosion classification in categories 1A, 1B and 1C is subject to some interpretation of the experimental results. Also, several oral LD_{50} values are available and these cluster around the critical value of 300 mg/kg that differentiates Acute Tox. category 3 from category 4. In this case, the value chosen may also depend on whether *anhydrous lithium hyd*roxide is used as the basis or the *monohydrate*.

5.1.3. Approaches to evaluating Classification and Labelling Inventory data

In the light of the problems described above, an approach to evaluate the Inventory data has been developed on the basis of a similar approach applied for components of metal-working fluids([13]). This approach prioritises the entries as follows:

- Harmonised classification.
- Classification and labelling information from a 'lead dossier' submitted under REACH([14])('Joint Entries' column ticked; this represents the information submitted by the lead company of a joint submission).
- The next highest priority is assigned to the entry with the highest number of notifiers.
- If the number of notifiers is not given, the most conservative H-statements were chosen (i.e. those representing the highest hazard).

5.1.4. Justification

Harmonised classifications according to Annex VI of the CLP Regulation have the highest priority since these have been established by the competent authorities of EU Member States. However, they may be overruled by a stricter classification from a 'joint entry'. These notifications from the lead dossier of a joint submission ('joint entries' in the C & L Inventory) in the REACH registration process are assumed to a) include the most recent (eco-) toxicological data generated for substance registration and b) involve some form of discussion in the consortia responsible for registration. Data may have been used that were previously unavailable, e.g. because they represent confidential information or because they were only generated to meet REACH information requirements. These data from different companies involved in the joint registration process were then discussed and – ideally – a common classification was reached (although there are possibilities for a company to opt out). In fact, there are cases, where the 'joint entry' classification is more robust than the harmonised

([13]) Described (in German) in: http://www.kss-komponenten.de/PDF/Erlaeuterungen_Formblaetter.pdf

([14]) Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) classification, since the information used is more up-to-date.

A typical example is shown in Figure 4, where the aquatic chronic classification from the ‘joint entry’ is stricter (aquatic chronic 2) than the harmonised classification (aquatic chronic 3) for the substance *isoprene* (CAS number: 78-79-5); information retrieved in August 2014; only the harmonised and the diverging ‘joint entry’ classification are shown).

Figure 4: Screenshot of selected information from the C & L Inventory for *isoprene*

Harmonised classification

Harmonised classification - Annex VI of Regulation (EC) No 1272/2008 (CLP Regulation)

General Information

Index Number	EC Number	CAS Number	International Chemical Identification
601-014-00-5	201-143-3	78-79-5	isoprene (stabilised) 2-methyl-1,3-butadiene

ATP Inserted / Updated: CLP00
CLP Classification (Table 3.1)

Classification		Labelling			Specific Concentration limits, M-Factors	Notes
Hazard Class and Category Code(s)	Hazard Statement Code(s)	Hazard Statement Code(s)	Supplementary Hazard Statement Code(s)	Pictograms, Signal Word Code(s)		
Flam. Liq. 1	H224	H224		GHS02 GHS08 Dgr		Note D
Muta. 2	H341	H341				
Carc. 1B	H350	H350				
Aquatic Chronic 3	H412	H412				

‚Joint entry‘ classification

Classification		Labelling			Specific Concentration limits, M-Factors	Notes	Classification affected by Impurities / Additives	Additional Notified Information	Number of Notifiers	Joint Entries	View
Hazard Class and Category Code(s)	Hazard Statement Code(s)	Hazard Statement Code(s)	Supplementary Hazard Statement Code(s)	Pictograms, Signal Word Code(s)							
Flam. Liq. 1	H224	H224		GHS02 GHS09 GHS08 Dgr				IUPAC Names	55	✔	
Muta. 2	H341	H341									
Carc. 1B	H350	H350									
Aquatic Chronic 2	H411	H411									

In such a case, it appears more meaningful to use the stricter classification from a ‘joint entry’.

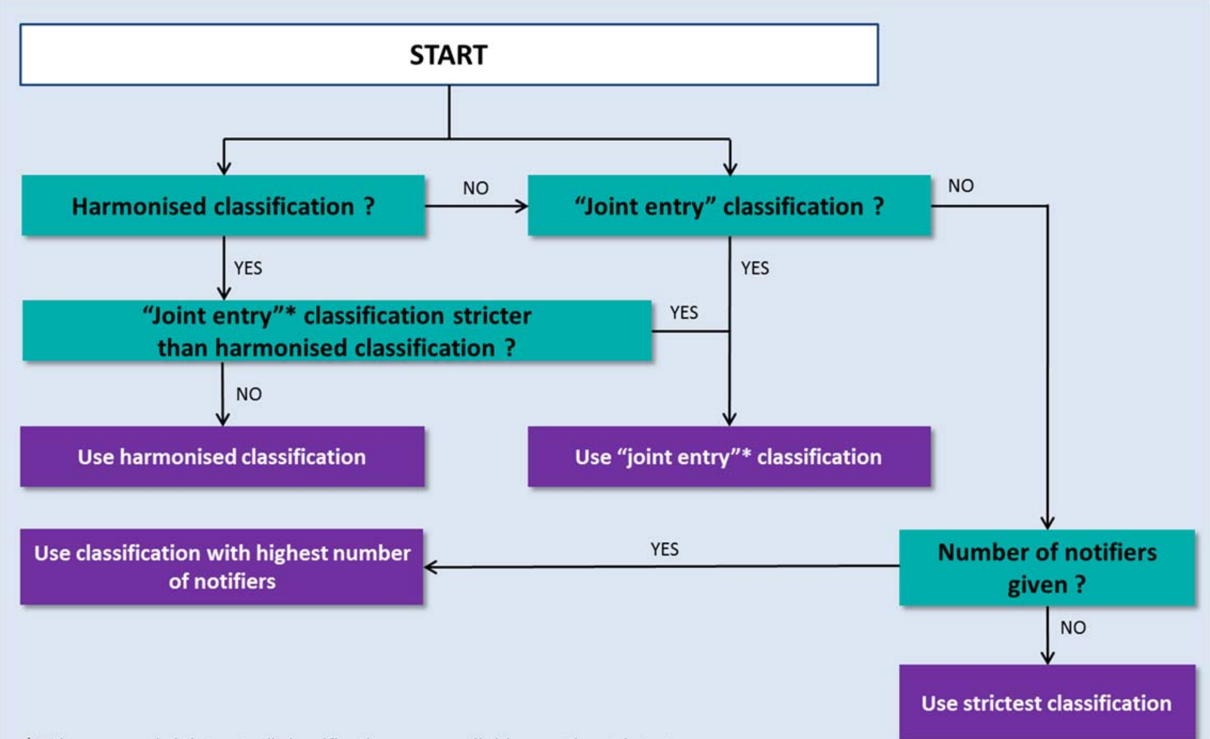
Extending the example presented above to chemicals covered by the indicator ‘Production of toxic chemicals’, we have recently shown that 37 out of 119 substances had a stricter ‘joint entry’ classification compared to the harmonised classification for human health endpoints and 29 of these were classified for at least one additional endpoint not covered by the harmonised classification. Additional analyses suggested that these classifications for additional endpoints sometimes resulted from experimental studies performed to fulfil REACH requirements (Oltmanns et al., 2014). These findings strongly corroborate the suggestion that ‘joint entry’ classifications may indeed provide more up-to-date information than harmonised classifications in some cases.

When neither a harmonised classification nor a ‘joint entry’ is available, the procedure is simply based on a ‘majority rule’ in that the classification provided by the highest number of notifiers is used.

The last level in the hierarchy applies to cases, where no information on the number of notifiers is provided. This should only relate to few cases and a worst case assumption is made, i.e. that the most conservative hazard statement is the correct one.

The overall decision tree is shown in the following figure. Note that a comparison of both the harmonised classification and ‘joint entry’ classifications is required when both are available.

Figure 5: **Decision tree for selection of data from the C & L Inventory**



** When several „joint entry" classifications are available, use the strictest one.*

5.2. Assigning hazard statements to toxicity classes

Once the H-statements are retrieved, they need to be assigned to the toxicity classes A-E of the indicator 'Production of toxic chemicals' (see Chapter 4). Assignment of hazards according to the CLP Regulation to classes A-E basically follows the procedures outlined above and uses the translation table provided in Annex VII of the CLP Regulation. Full details are provided in Annex 1.

For acute toxicity, a minimum classification is usually derived by 'automatic' translation that needs to be checked against the actual toxicity data. The reason for this requirement lies in the fact that the new CLP classification criteria have somewhat different class boundaries than the old system according to Directive 67/548/EEC (Dangerous Substances Directive, DSD). However, acute toxicity hazards may only lead to classes C-E (see Annex 1) and the acute toxicity data for substances assigned to class 'C' or higher for another reason (e.g. skin sensitizers (class B) or carcinogens (class A)) need not be checked for accuracy of the acute toxicity classification. In all other cases, acute toxicity data from the registration dossiers (as contained in ECHA CHEM([15])) or – in rare cases – from reliable reviews were checked against classification.

Classification information for the 'Production of environmentally harmful chemicals' was evaluated in a similar way and the assignment to impact classes is presented in Annex 2. For environmental endpoints translation is straightforward and no specific checks are required. However, a much higher emphasis is put on chronic aquatic effects under the CLP Regulation and information from the C & L Inventory may well reflect this fact.

([15]) See http://echa.europa.eu/web/guest/information-on-chemicals/registered-substances

5.3. Changes in class assignment following the revision

The number of PRODCOM entries related to toxic chemicals and the assignment to classes A-E is shown in Table 5.

Table 5: Number of products of toxic chemicals in PRODCOM per toxicity class

Class	Number of products
A	34
B	30
C	30
D	49
E	41
Sum	184

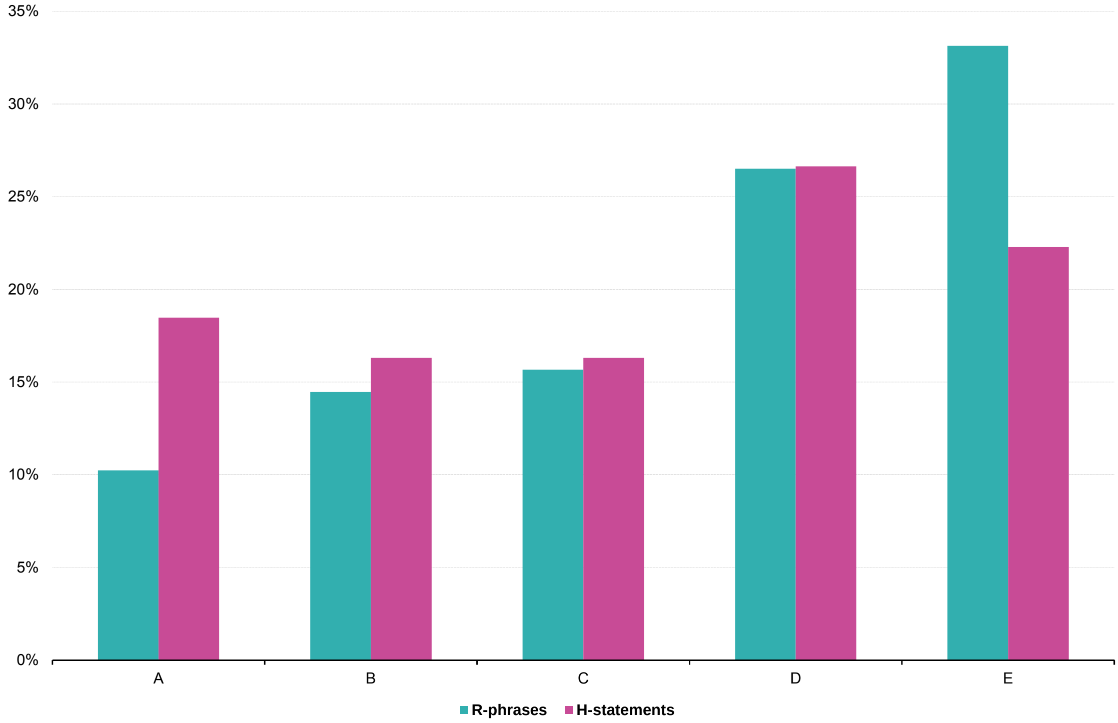
The 184 PRODCOM entries with toxic properties make up the indicator ‘Production of toxic chemicals’. The 184 PRODCOM entries and the CAS numbers of substances assessed for each entry are shown in Annex 4, differentiated by toxicity class.

Note that because a single PRODCOM entry may relate to different individual chemicals, the total number of substances is higher (184) than the number of PRODCOM entries (130) identified in Table 4 (shown in Chapter 4).

The assessment approach, as described above, focussed on harmonised classifications as well as classifications from REACH registration dossiers (‘joint entry’ classifications), since these are considered more reliable than classifications from other notifications. As a consequence, about 94 % of the substances were assessed on the basis of a harmonised classification or a ‘joint entry’ classification. The remaining substances were assessed on the basis of the highest number of notifications (about 6 %), because harmonised and ‘joint entry’ classifications were not available. The hazard information for the substances evaluated for the indicators can therefore be considered very reliable.

The extraction of classifications (H-statements) from the C & L Inventory resulted in some changes in class assignment compared to previous evaluations (R-phrases according to the DSD). Overall, a change is observed for 28.5 % of the substances evaluated with 26.1% showing a higher and 2.4 % showing a lower hazard class under the new evaluation. The changes in the new 2013 evaluation are shown in the following figure for the indicator ‘Production of toxic chemicals’.

Figure 6: Changes in class assignment after inclusion of C & L Inventory data ('Production of toxic chemicals'): percent of substances assigned to each toxicity class



While the previous distribution (R-phrases according to DSD) is characterised by an increase in the percentage of substance with decreasing toxic hazard class (from about 10 % in class A to about 33 % in class E), the new evaluation leads to a more even distribution among the classes. In other words, there is a clear shift from the less hazardous class E to the more hazardous classes and particularly to class A, the one associated with the highest hazard. Several reasons for these changes can be identified and in some cases require a detailed assessment, but the following reasons appear to be the most important ones:

- The 'old' risk phrases and the resulting class assignments were out-dated. As an example, four different *lead* compounds were not classified for their reproductive toxicity, but rather for their comparatively low acute toxicity. All these four compounds moved from class E to class A. For *lead*, as for many other metals, the out-dated classification might also relate to the fact that these substances sometimes do not have a harmonised classification under their substance name with the corresponding CAS or EC number, but are rather classified as summary entries (e.g. '*lead* compounds with the exception of those specified elsewhere in this Annex', the latter referring to Annex VI of the CLP Regulation). About one fourth of all increases in hazard class relate to metals and their compounds. Nonetheless, out-dated classifications also relate to many other, clearly identified substances. For example, *toluene* was previously assigned to class E based on R20, while it has a harmonised classification for suspected reproductive toxicity (H361), leading to class B. About 45 % of the substances with a higher hazard in 2013 than before have a harmonised classification that was either not properly recorded in previous evaluations or was updated in between.
- The classification from registration dossiers ('joint entry') is stricter than the previous (harmonised or not) classification. In some of these cases, the basis for the stricter classification (e.g. for repeated dose toxicity) is not entirely clear and would require an analysis of the Chemical Safety Report. In other cases, e.g. for some substances causing severe eye damage or skin sensitization, the new data appear to have been generated due to REACH (e.g. studies performed in 2009 and 2010). However, some 'joint entry' classifications that are stricter than

existing harmonised classifications do not rely on new study reports, but rather appear to include a new assessment of existing data, resulting in a new classification. This issue was assessed in more detail by Oltmanns et al. (2014). Overall, more than 20 % of all substances with a stricter toxic hazard class are assigned to this class due to ‘joint entry’ classifications.

- In the absence of a risk phrase, an occupational exposure limit value (German ‘MAK’ value) was used in the previous assessment. In the new evaluation, a hazard statement was available in the C & L Inventory for many of these substances and was responsible for the change. Note that while this availability of a classification primarily led to increases in the toxic hazard class (about 10 % of all substances with increases), it was also responsible for decreases in the toxic hazard class (50 % of all substances with decreases).
- Overall, this evaluation shows that:
- an update of the classification information was urgently required, since the new evaluation corrected some errors and now includes more recent information,
- REACH led to new data resulting in classification for additional endpoints and/or to a stricter classification than the one previously available (harmonised or not),
- the CLP Regulation itself provided new information, since the C & L Inventory contains data for substances for which no classification could be previously located,
- a trend towards higher toxic hazards results from this up-to-date extraction of classification data from the C & L Inventory.

6 Update of the indicator

6.1. Production of toxic chemicals according to H-statements: Production volume and share of toxicity classes

The basic chemical industry in Europe has seen a decrease of the production volume in 2013, another dip following the short growth period of 2010 and the subsequent decrease in 2011 and 2012. The production volume in 2013 is the second lowest since 2004 when reporting for EU-28 started. For EU-15 and EU-28, the following details can be reported:

6.1.1. EU-28

The total production of chemicals amounted to approximately 355 million tonnes in the first reporting year 2004. The production rose to 371 million tonnes in 2007 and then abruptly declined to 296 million tonnes in 2009 due to the economic crisis. After a rebound in 2010 and a decrease in 2011 and 2012, the 2013 production is about 322 million tonnes, the second lowest production figure since reporting started in 2004 (Figure 7).

6.1.2. EU-15

The EU-15 time series started in 1996 with a production volume of 260 million tonnes and increased steadily until 2007 with a production volume of 316 million tonnes. Because of the recession, the production strongly decreased to a volume of 252 million tonnes in 2009. After a rebound to about 293 million tonnes in 2010 and 2011, the production volume is down again to 276 million tonnes in 2012 and to 273 million tonnes in 2013. This production volume represents the second lowest volume since 1997 (Figure 7).

Figure 7 also details the development of the production volume by toxicity class. Like the general decline in the overall production volume we also observe the decline in the different toxicity classes.

One main reason for the general decline is the lower demand for plastics (not covered in this figure), which is reflected in the lower demand of the upstream chemicals *(benzene, vinyl chloride, chlorine, caustic soda etc.)*. This is especially obvious for PVC production which strongly relies on the construction sector. In addition to the lower local demand, the declining production may also be due to higher energy prices and to shifts to other regions, especially the USA and East Asia. As we have noticed a shift in production from the USA to Europe between 2000 and 2007 caused by the shortage of *natural gas*, the current reversal may be partly characterised as a sort of 'normalisation'.

Figure 7: Development of the total production in EU-15 and EU-28: production volume (million tonnes per annum) by toxicity classes (based on H-statements)

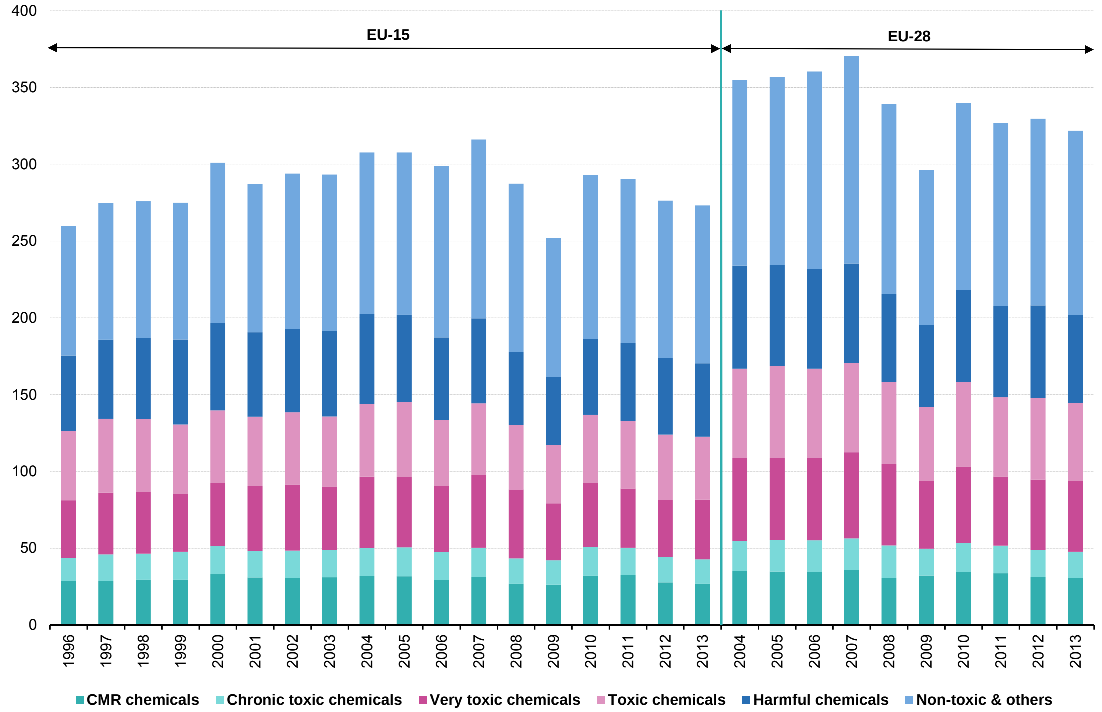


Figure 8 shows the development in the toxicity share. The differences from year-to-year are very small. Over time, an overall decline in the share of CMR chemicals and in the share of all five toxicity classes can be assumed (details in Table 6).

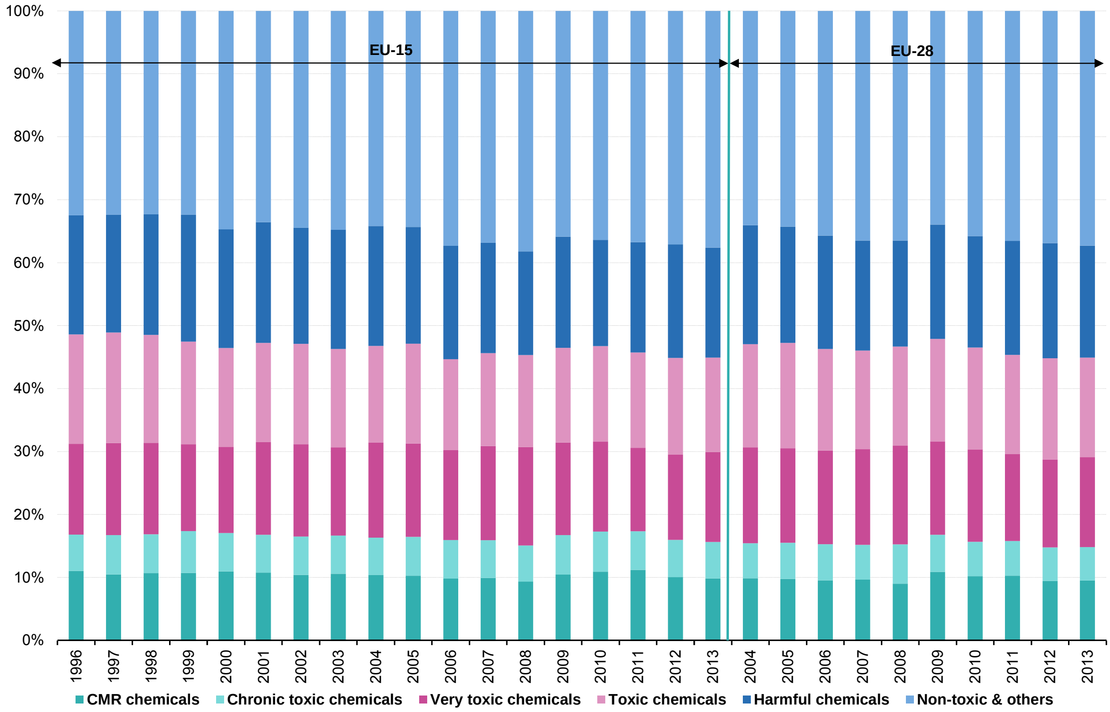
Table 6: Comparison of the shares of CMR and 'all toxic chemicals' in EU-15 and EU-28 from 2004 to 2013

	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013
CMR chemicals (class A)										
EU-15	10.4%	10.3%	9.8%	9.9%	9.3%	10.5%	10.9%	11.2%	10.1%	9.8%
EU-28	9.9%	9.8%	9.5%	9.7%	9.0%	10.9%	10.2%	10.3%	9.5%	9.5%
All toxic chemicals (classes A-E)										
EU-15	65.8%	65.7%	62.7%	63.2%	61.8%	64.1%	63.6%	63.3%	62.9%	62.8%
EU-28	66.0%	65.7%	64.3%	63.5%	63.5%	66.0%	64.2%	63.5%	63.1%	62.7%

The table shows a general decline in 'all toxic chemicals' from 66 % in 2004 to 63 % in 2013. For 'CMR' chemicals, figures decline from 10.4 % to 9.8 % for EU-15 and from 9.9 % to 9.5 % for EU-28.

For a general assessment of a 'trend', the variability of the production data and also the production share is too high. The lowest share of 'CMR' chemicals as well as the sum of all toxicity classes can generally be observed in 2008.

Figure 8: **Development of the total production in EU-15 and EU-28: share according to toxicity classes (based on H-statements)**



6.2. Production of toxic chemicals according to R-phrases: Production volume and share of toxicity classes

The following figures show the development of the production volume by toxicity classes and the share of the toxicity classes based on R-phrases. Compared to the figures based on H-statements, results are very similar and differ only in detail.

Figure 9: **Development of the total production in EU-15: production volume (in 1 000 tonnes per annum) according to toxicity classes (based on R-phrases)**

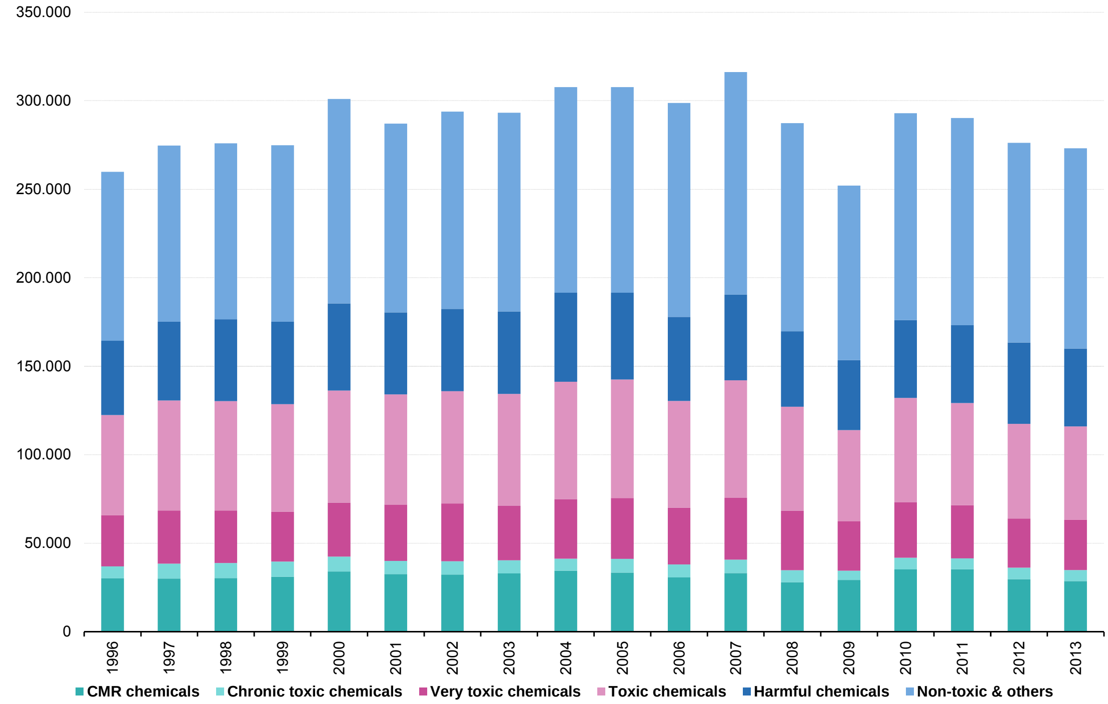
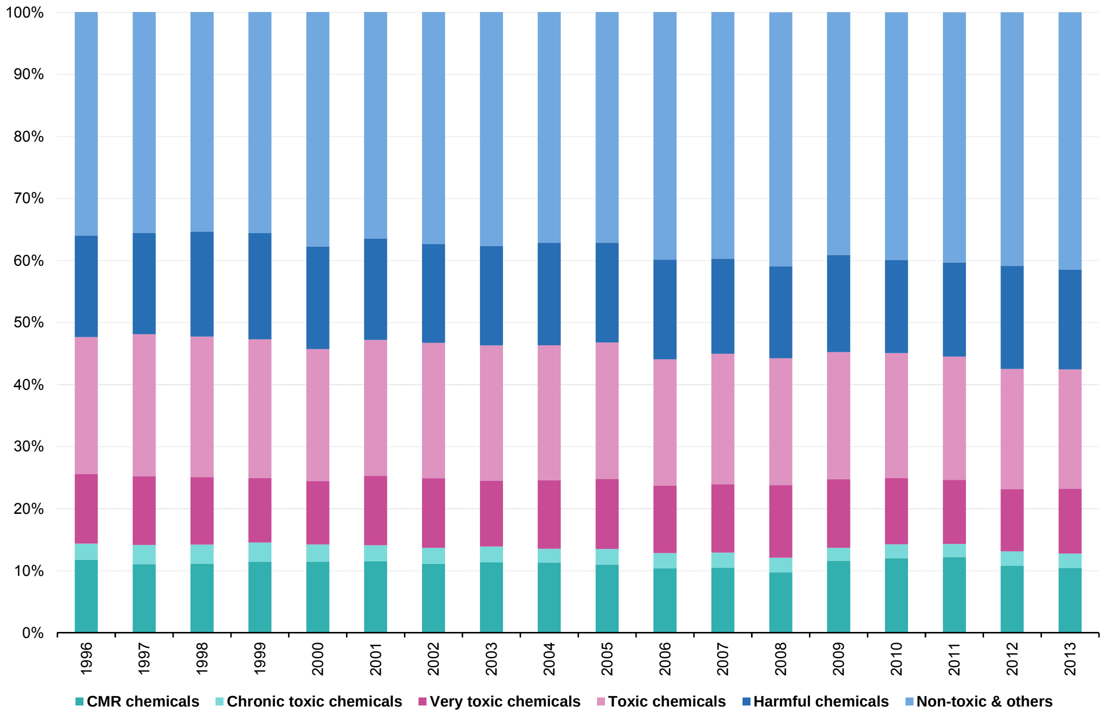


Figure 10: **Development of the total production in EU-15: share according to toxicity classes (based on R-phrases)**



6.3. Production of toxic chemicals in EU-15: Comparison of results from 'H-statement aggregation' and 'R-phrases aggregation'

The result for the indicator 'Production of toxic chemicals' is now available for EU-15 for the two classification schemes, the old one according to R-phrases and the new one according to H-statements.

The revision of the indicator system described in detail above led to a more even distribution of chemicals among the toxicity classes based on H-statements when compared with those based on R-phrases. Figure 11 shows the number of chemicals in each toxicity class (the same data with the percentages of substances were already presented in Figure 6) and again shows the higher number of e.g. CMR chemicals based on H-statements when compared against the assessment based on R-phrases as well as the lower number of 'harmful' chemicals.

These data suggest that the volume of CMR chemicals might increase and the volume for 'harmful' chemicals might decrease. However, the production volumes shown in Figure 12 identify an opposite trend. This can be explained by the fact that one high volume chemical has been re-assessed as being a suspected CMR substance rather than a confirmed CMR substance, and many lower volume chemicals have been promoted to the CMR class. In total, this has resulted in a lower volume-based share of CMR chemicals in relation to the total production of chemicals.

The contrary has happened for the 'harmful' chemicals. The number of chemicals classified as harmful has declined, but the total volume of these chemicals has increased.

The quality of the indicator has improved: The distribution by numbers of the five toxicity classes is now more levelled (see Figure 11). Especially, the number of chemicals in the CMR class shows a better coverage. For the distribution by volume a slightly better distribution can be observed.

Figure 11: Number of chemicals per toxicity class based on R-phrases and based on H-statements

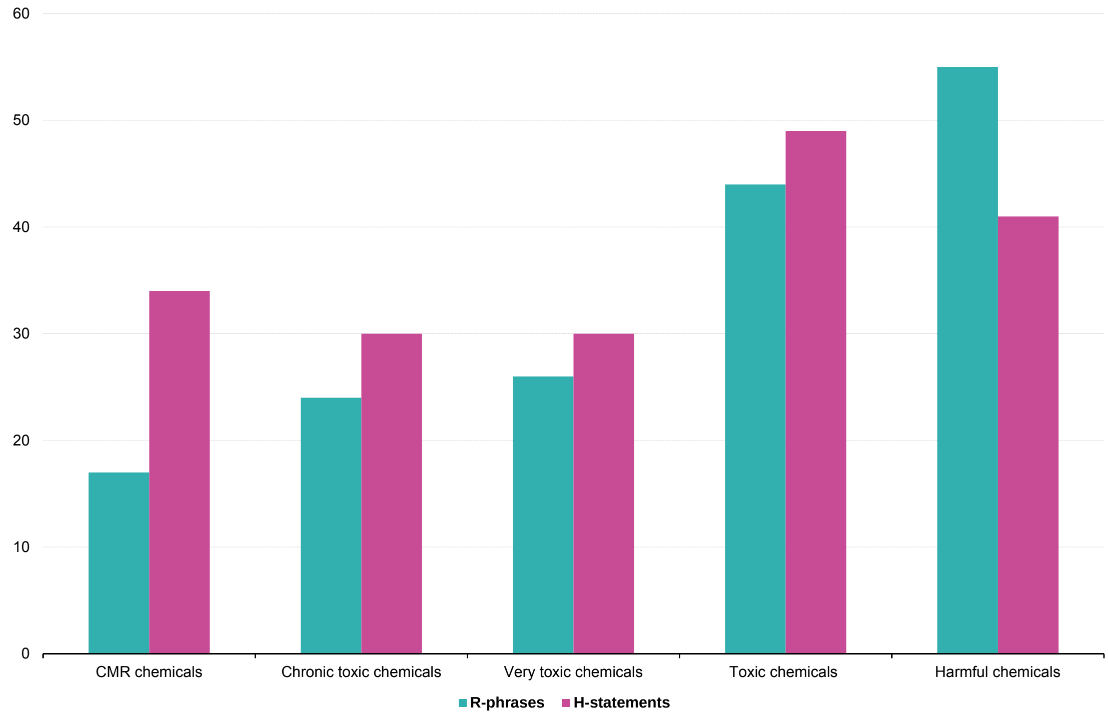
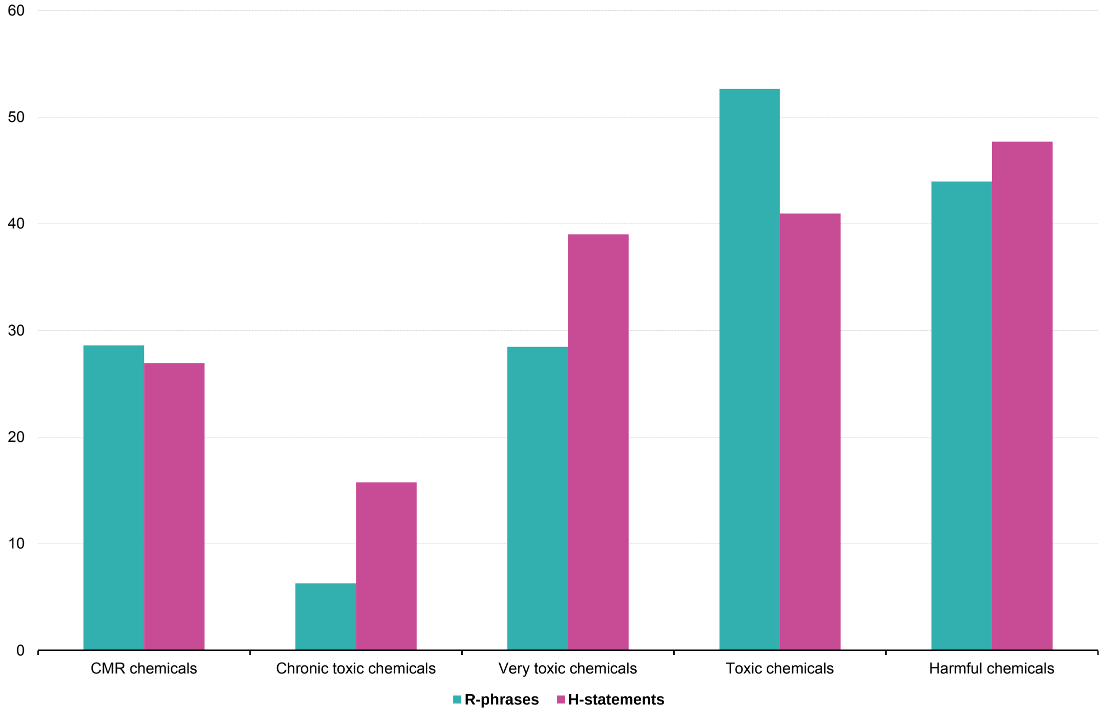


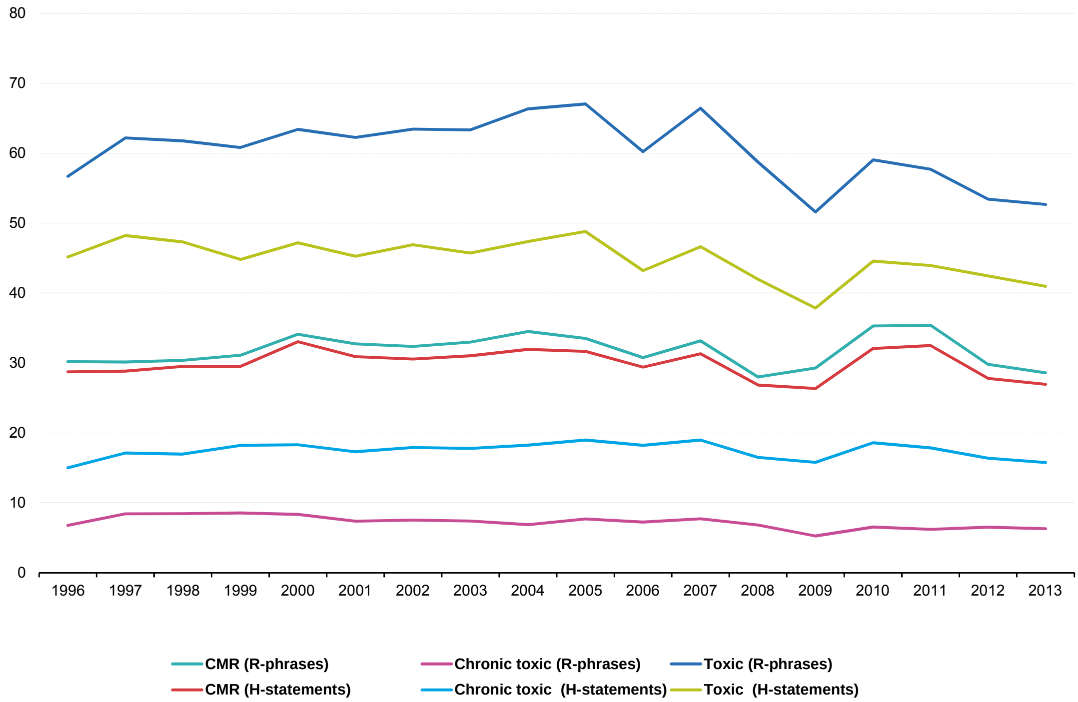
Figure 12: **Results for 'Production of toxic chemicals' according to the two classification schemes for the year 2013: production volume in million tonnes per annum**



The following figures show a comparison in the time series of the toxicity classes for the two schemes (R-phrases and H-statements), displaying the three toxicity classes: 'CMR chemicals', 'chronic toxic' and 'toxic' (classes A, B and D).

All three classes are displayed for R-phrases and H-statements for the production volume (Figure 13) and production share (Figure 14) for easier identification of the changes between the toxicity classes.

Figure 13: **Comparison for 'Production of toxic chemicals – EU-15' according to the H-statements and R-phrases classification scheme: production volume in million tonnes per annum**



The production volume figure shows the differences between the two classification schemes and their development over time. The CMR graphs for the two schemes are nearly identical. The CMR R-phrases tends to be higher especially during 'growth' periods. Both graphs are also influenced by the 'up-and-downs' of the general production. This is more visible for 'toxic' R-phrases where this effect is even more pronounced.

The following figure shows the share of the production volumes. The graphs are more even as the production variability is filtered out. A look at possible trends shows different effects:

1. 'CMR chemicals': no trend observable (R-phrase and H-statements).
2. 'Chronic toxic': no trend observable (R-phrase and H-statements).
3. 'Toxic': steady decrease for aggregation by R-phrases. For the aggregation by H-statements the decrease is visible until 2007, afterwards constant.

Figure 14: Comparison for 'Production of toxic chemicals – EU-15' according to H-statements and R-phrases classification scheme: production share

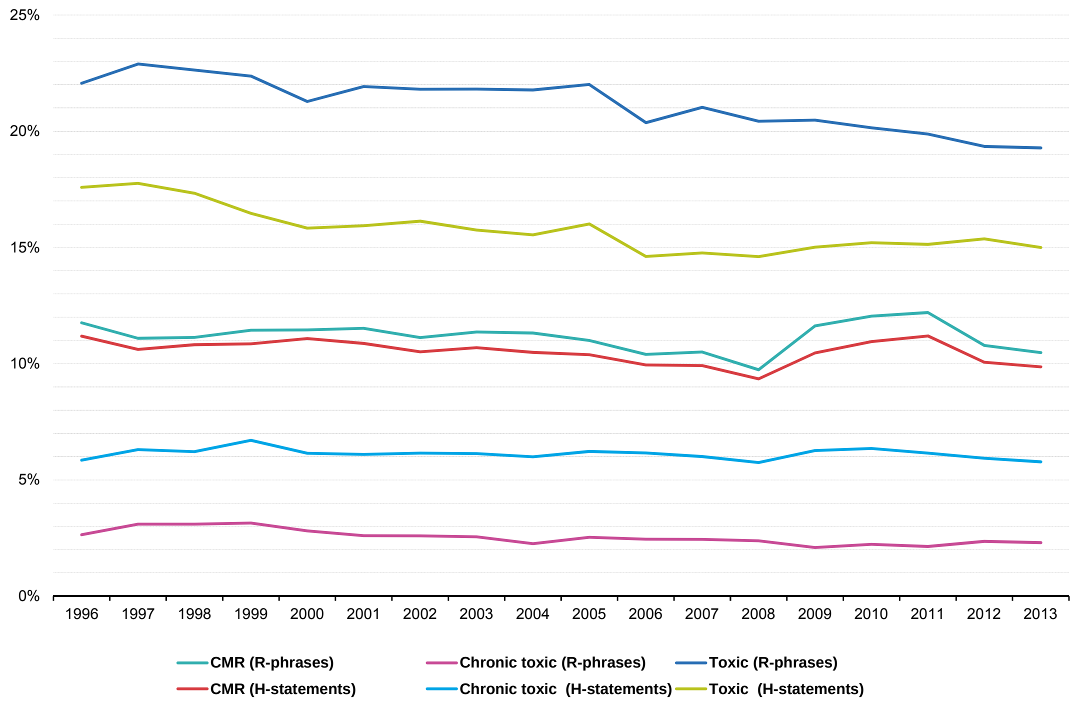


Table 7 shows the decrease / increase for the toxicity classes according to the two schemes. The class 'non-toxic & others' is the counterpart of the 'sum of the five toxicity classes'. The figure of about 5 % for the class 'non-toxic & others' indicates that this class is increasing during the period, while the five toxicity classes are decreasing. For both schemes the decrease / increase is nearly the same. For the toxicity classes 'CMR chemical', 'chronic toxic' and 'very toxic' (classes A-C) the changes during the period are small (0.50 to 0.79 percentage points) and the differences between the two schemes during the period are mostly negligible.

The biggest change during the period is calculated for the 'toxic chemicals' (class D, both schemes) and for the 'harmful chemicals' (class E, for H-statement scheme only). Both classes together yield -3.9 percentage points for R-phrases and -4.2 percentage points for H-statements.

Table 7: Change in production share in EU-15 for toxicity classes according to R-phrases and H-statements

Class	R-phrases*	H-statements*
CMR chemicals (class A)	-0.62 %	-0.75 %
Chronic toxic chemicals (class B)	-0.79 %	-0.53 %
Very toxic chemical (class C)	-0.62 %	-0.50 %
Toxic chemicals (class D)	-3.61 %	-2.76 %
Harmful chemicals (class E)	-0.27 %	-1.44 %
Non-toxic & others	4.80 %	4.87 %

* Negative values indicate decreases from 1997 to 2013

6.4. Consumption of toxic chemicals: Results for aggregation by H-statements

The production indicators discussed so far only address chemical production within the EU. However, chemicals produced in the EU are also exported to other countries and chemicals produced outside the EU are also imported into the EU. These flows are addressed by the consumption indicators.

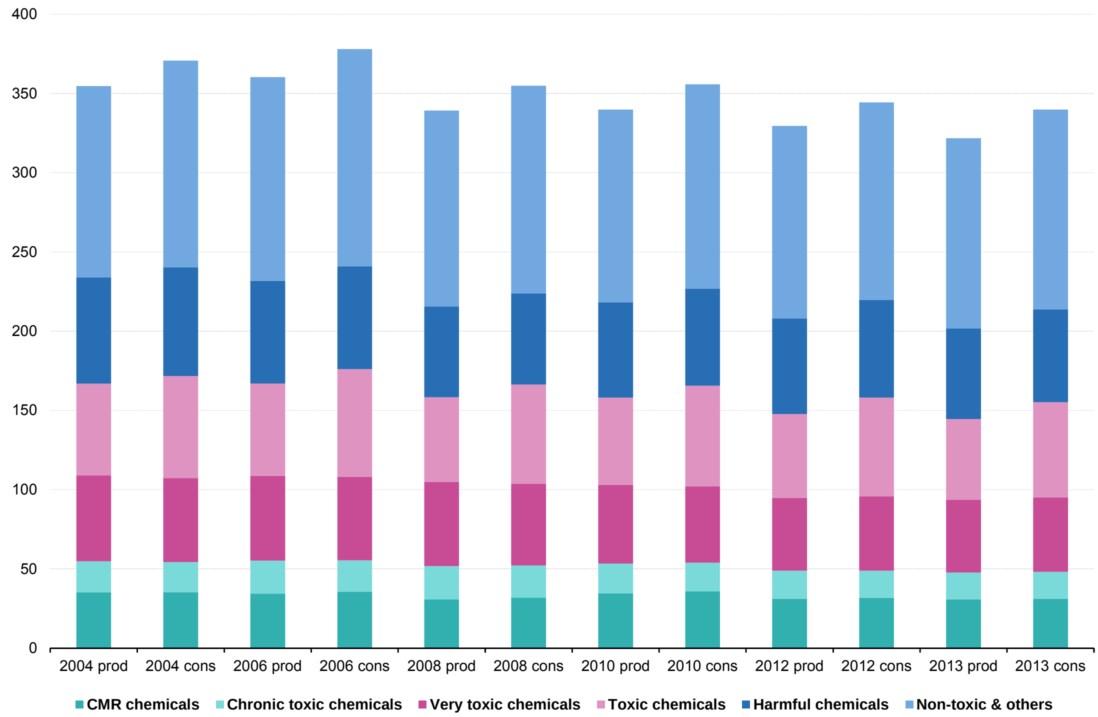
The consumption of chemicals is calculated according to the equation:

Consumption = production + imports - exports

Production figures are taken from PRODCOM, while import and export figures are taken from COMEXT (Eurostat's reference database for international trade).

Figure 15 shows the consumption and production figures according to H-statements for some selected years for EU-28.

Figure 15: Consumption and production of chemicals by toxicity class (EU-28 based on H-statements, production volume in million tonnes per annum)



The data show that the consumption in the EU-28 is higher than the production. The EU-28 is a net importer of chemicals. The distribution of the toxicity classes is very similar in the consumption and the production figures.

Figure 16 shows the data for 2013 in detail. Only the classes of 'non-toxic & others' and 'toxic chemicals' show a significant contribution to net imports, while the four other classes do not.

Figure 16: **Consumption and production of chemicals (in million tonnes per annum) by toxicity class (EU-28 based on H-statements, 2013)**

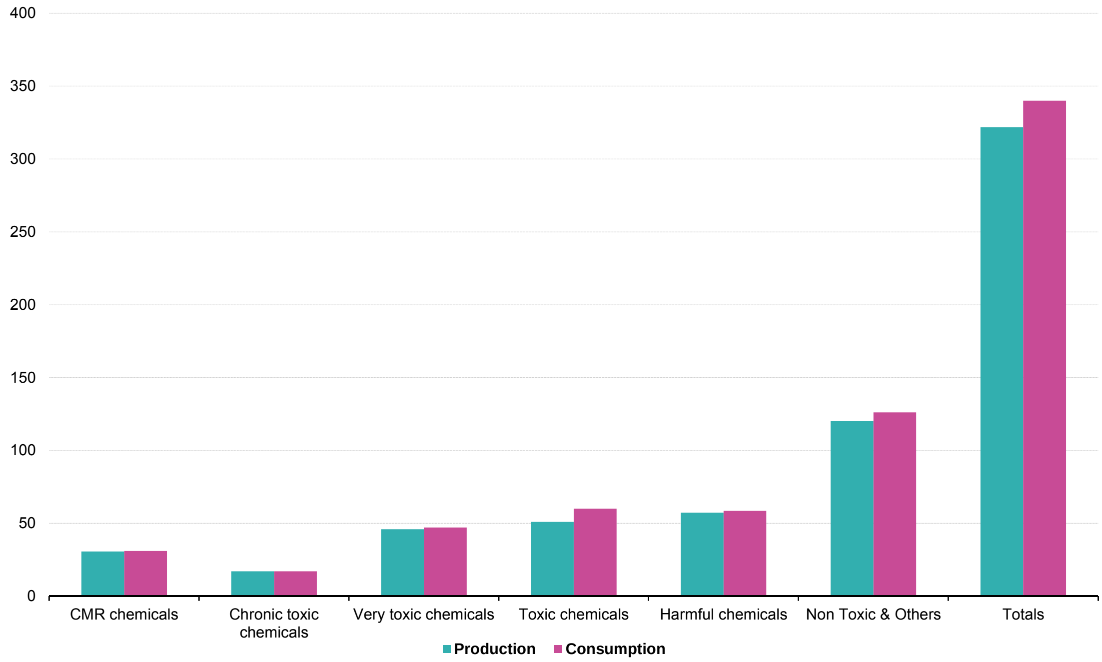
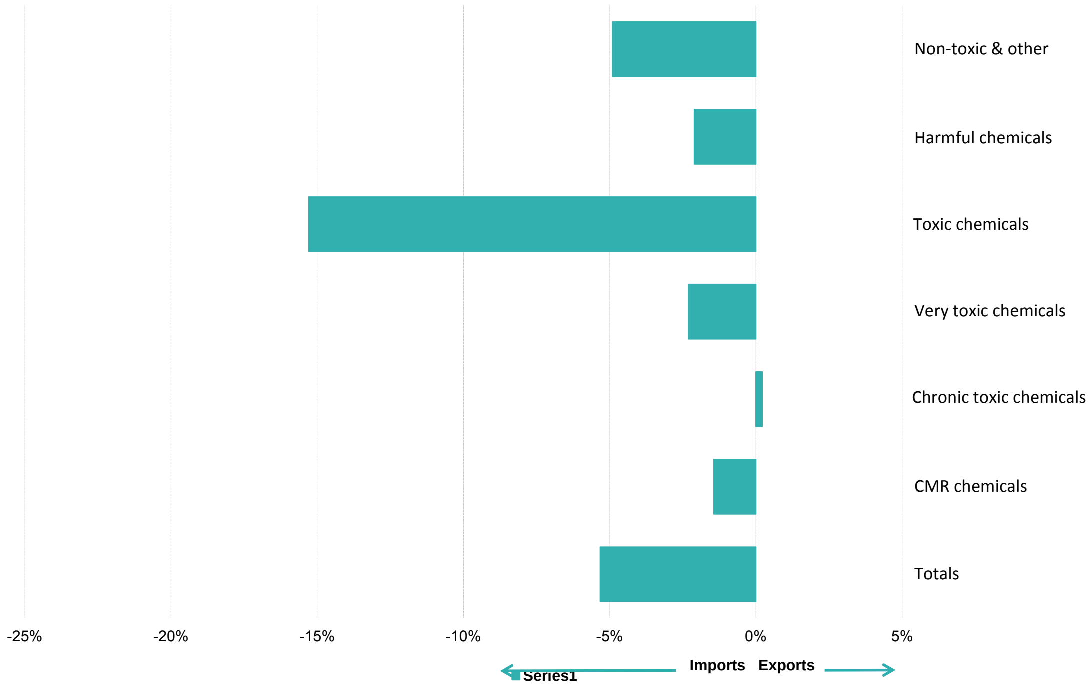


Figure 17 shows the net import (import - export) over consumption for each toxicity class.

A detailed look at the toxicity classes shows that the contributions to the overall 5 % net imports are distributed unevenly. For the ‘chronic toxic chemicals’ we observe net exports. The contributions of ‘harmful chemicals’ (2 %), ‘very toxic chemicals’ (2 %) and ‘CMR chemicals’ (1.4 %) are significantly lower than the average. These deficits are made up by the ‘toxic chemicals’ with a net import of about 15 %. The ‘toxic chemicals’ consumption in 2013 is 60 million tonnes and the net import of ‘toxic chemicals’ is 9.2 million tonnes (approximately 15 %).

Figure 17: Share of net imports on consumption of chemicals by toxicity class (EU-28 based on H-statements, production volume 2013)



7 References

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European Union Risk Assessment Report: 1,3-Butadiene. 1st Priority List, Vol. 20
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Guidance on the Application of the CLP Criteria. Version 3.0 - November 2012
Helsinki, Finland

Oltmanns, J.; Bunke, D.; Jenseit, W.; Heidorn, C. (2014)
The impact of REACH on classification for human health hazards
Regulatory Toxicology and Pharmacology, 70, 474-481

8 Additional resources

8.1. Eurostat information

Publications

- Sustainable development in the European Union – 2015 monitoring report of the EU Sustainable Development Strategy (2015): http://ec.europa.eu/eurostat/web/products-statistical-books/-/KS-GT-15-001
- Statistics explained – Chemicals production statistics: http://ec.europa.eu/eurostat/statistics-explained/index.php/Chemicals_production_statistics
- Eurostat Pocketbook: Energy, transport and environment indicators (2015): http://ec.europa.eu/eurostat/en/web/products-statistical-books/-/KS-DK-15-001
- Environmental statistics and accounts in Europe – Statistical book (2010): http://ec.europa.eu/eurostat/web/products-statistical-books/-/KS-32-10-283

Main tables

- Sustainable development indicators public health: http://ec.europa.eu/eurostat/web/sdi/indicators/public-health -> Index of production of toxic chemicals, by toxicity class: http://ec.europa.eu/eurostat/tgm/table.do?tab=table&plugin=1&language=en&pcode=tsdph320
- Environment - Hazardous substances: http://ec.europa.eu/eurostat/web/environment/hazardous-substances/main-tables -> Production of environmentally harmful chemicals, by environmental impact class: http://ec.europa.eu/eurostat/tgm/table.do?tab=table&init=1&language=en&pcode=ten00011&plugin=1
- Source data for tables and figures of the indicators: http://ec.europa.eu/eurostat/statistics-explained/index.php/Chemicals_production_statistics -> Source data for tables and figures (MS Excel) - > Chemicals production statistics: tables and figures
- PRODCOM data:
  - All data: http://ec.europa.eu/eurostat/web/prodcom/data/excel-files-nace-rev.2
  - Database: http://ec.europa.eu/eurostat/web/prodcom/data/database

8.2. External links

European Chemicals Agency (ECHA)

- Information on registered substances: http://echa.europa.eu/information-on-chemicals/registered-substances
- Classification and Labelling Inventory: http://echa.europa.eu/information-on-chemicals/cl-inventory-database

9 Annexes

9.1. Annex 1: Assignment of risk phrases and hazard statements to toxic impact classes

The following table shows the assignment relevant for the indicator ‘Production of toxic chemicals’. It basically follows the old assignment and uses the translation table provided in Annex VII of Regulation (EC) No 1272/2008 to assign hazard statements to toxic impact classes (A-F). For acute toxicity endpoints, classification criteria have change and a minimum classification as well as a higher classification is possible. New classes (Skin Corr. 1C) are assigned to an impact class and justification is provided below.

Table 8: Summary of the assignment to toxic impact classes

Classification under Directive 67/548/EEC	Classification under Regulation (EC) No 1272/2008		Classes		Rationale/ Remarks
	Hazard Class/ Category	Hazard statement	Old	New	
Xn; R20 (gas)	Acute Tox. 4	H332	E	E/D	Data may overrule minimum classification
Xn; R20 (vapour)	Acute Tox. 4	H332	E	E/D	
Xn; R20 (dust/mist)	Acute Tox. 4	H332	E	E	
Xn; R21	Acute Tox. 4	H312	E	E/D	
Xn; R22	Acute Tox. 4	H302	E	E/D	
T; R23 (gas)	Acute Tox. 3	H331	D	D/C	
T; R23 (vapour)	Acute Tox. 2	H330	D	D	
T; R23 (dust/mist)	Acute Tox. 3	H331	D	D/C	
T; R24	Acute Tox. 3	H311	D	D/C	
T; R25	Acute Tox. 3	H301	D	D/C	
T+; R26 (gas)	Acute Tox. 2	H330	C	C	Higher classification for acute toxicity impossible
T+; R26 (vapour)	Acute Tox. 1	H330	C	C	
T+; R26 (dust/mist)	Acute Tox. 2	H330	C	C	
T+; R27	Acute Tox. 1	H310	C	C	
T+; R28	Acute Tox. 2	H300	C	C	
R33	STOT RE 2	H373	D	D	
C; R34	Skin Corr. 1B	H314	D	D	Skin Corr. 1C (H314): D
C; R35	Skin Corr. 1A	H314	C	C	

Classification under Directive 67/548/EEC	Classification under Regulation (EC) No 1272/2008		Classes		Rationale/ Remarks
	Hazard Class/ Category	Hazard statement	Old	New	
Xi; R36	Eye Irrit. 2	H319	E	E	
Xi; R37	STOT SE 3	H335	E	E	
Xi; R38	Skin Irrit. 2	H315	E	E	
T; R39/23	STOT SE 1	H370	D	D	Analogy with acute toxicity
T; R39/24	STOT SE 1	H370	D	D	
T; R39/25	STOT SE 1	H370	D	D	
T+; R39/26	STOT SE 1	H370	C	C	
T+; R39/27	STOT SE 1	H370	C	C	
T+; R39/28	STOT SE 1	H370	C	C	
Xi; R41	Eye Dam. 1	H318	D	D	
R42	Resp. Sens. 1	H334	B	B	
R43	Skin Sens. 1	H317	B	B	
Xn; R48/20	STOT RE 2	H373	D	D	
Xn; R48/21	STOT RE 2	H373	D	D	
Xn; R48/22	STOT RE 2	H373	D	D	
T; R48/23	STOT RE 1	H372	C	C	
T; R48/24	STOT RE 1	H372	C	C	
T; R48/25	STOT RE 1	H372	C	C	
R64	Lact.	H362	B	B	
Xn; R65	Asp. Tox. 1	H304	E	E	
R67	STOT SE 3	H336	E	E	
Xn; R68/20	STOT SE 2	H371	E	E	
Xn; R68/21	STOT SE 2	H371	E	E	
Xn; R68/22	STOT SE 2	H371	E	E	
Carc. Cat. 1; R45	Carc. 1A	H350	A	A	
Carc. Cat. 2; R45	Carc. 1B	H350	A	A	
Carc. Cat. 1; R49	Carc. 1A	H350i	A	A	
Carc. Cat. 2; R49	Carc. 1B	H350i	A	A	
Carc. Cat. 3; R40	Carc. 2	H351	B	B	
Muta. Cat. 1; R46	Muta. 1A	H340	A	A	Not in translation table
Muta. Cat. 2; R46	Muta. 1B	H340	A	A	
Muta. Cat. 3; R68	Muta. 2	H341	B	B	
Repr. Cat. 1; R60	Repr. 1A	H360F	A	A	
Repr. Cat. 2; R60	Repr. 1B	H360F	A	A	
Repr. Cat. 1; R61	Repr. 1A	H360D	A	A	
Repr. Cat. 2; R61	Repr. 1B	H360D	A	A	

Classification under Directive 67/548/EEC	Classification under Regulation (EC) No 1272/2008		Classes		Rationale/ Remarks
	Hazard Class/ Category	Hazard statement	Old	New	
Repr. Cat. 3; R62	Repr. 2	H361f	B	B	
Repr. Cat. 3; R63	Repr. 2	H361d	B	B	
Repr. Cat. 1; R60-61	Repr. 1A	H360FD	A	A	
Repr. Cat. 1; R60 Repr. Cat. 2; R61	Repr. 1A	H360FD	A	A	
Repr. Cat. 2; R60 Repr. Cat. 1; R61	Repr. 1A	H360FD	A	A	
Repr. Cat. 2; R60-61	Repr. 1B	H360FD	A	A	
Repr. Cat. 3; R62-63	Repr. 2	H361fd	B	B	
Repr. Cat. 1; R60 Repr. Cat. 3; R63	Repr. 1A	H360Fd	A	A	
Repr. Cat. 2; R60 Repr. Cat. 3; R63	Repr. 1B	H360Fd	A	A	
Repr. Cat. 1; R61 Repr. Cat. 3; R62	Repr. 1A	H360Df	A	A	
Repr. Cat. 2; R61 Repr. Cat. 3; R62	Repr. 1B	H360Df	A	A	

Substances classified as Skin Corr. 1C (H314) are also assigned to class ‘D’, since they are treated in the same way as those of category 1B in the context of qualitative risk characterisation according to ECHA Guidance IR & CSA, Part E (ECHA, 2012b).

9.2. Annex 2: Assignment of risk phrases and hazard statements to environmental impact classes

The following table shows the assignment relevant for the EPI ‘Production of environmentally harmful chemicals’. It basically follows the old assignment and uses the translation table provided in Annex VII of Regulation (EC) No 1272/2008 to assign hazard statements to toxic impact classes (A-E).

Table 9: Summary of the assignment to environmental impact classes

Classification under Directive 67/548/EEC	Classification under Regulation (EC) No 1272/2008		Classes	
	Hazard Class and Category	Hazard statement	Old	New
N; R50	Aquatic Acute 1	H400	E	E
N; R50-53	Aquatic Acute 1; Aquatic Chronic 1	H400; H410	A	A
N; R51-53	Aquatic Chronic 2	H411	B	B
R52-53	Aquatic Chronic 3	H412	C	C
R53	Aquatic Chronic 4	H413	D	D
R53 and log Kow 5.2-6.0	Aquatic Chronic 4	H413 and log Kow 5.2-6.0	A	A

Classification under Directive 67/548/EEC	Classification under Regulation (EC) No 1272/2008		Classes	
	Hazard Class and Category	Hazard statement	Old	New
R53 and (R45 or R46 or R48 or R60 or R61 or R62 or R63 or R64)	Aquatic Chronic 4	H413 and (H350 or H340 or H372 or H373 or H360 or H361 or H362)*	A	A
N; R59	Ozone	H420		

* According to the methodology, any of these human health hazard statements leads to class E, even if the substance is not classified for environmental hazards.

9.3. Annex 3: Assessing intermediates covered by the indicator

9.3.1. Background

The production- and consumption-based indicators do not provide information on the exposure related to the use of the chemicals covered by the indicator. Even an increased consumption of these chemicals does not necessarily result in increased exposure or increased risks for human health. In specific sectors, increased consumption can for example go along with improved risk management measures.

In addition, it has been questioned whether the indicators developed are actually relevant to exposure since many of the substances may primarily be used as intermediates, with little or no potential for exposure. An intermediate is a substance used in the manufacturing of another substance whereby the intermediate is itself transformed into that other substance.

This latter issue is the subject of the analysis presented in this annex and can be re-phrased in the key question: Are substances covered by the indicators primarily intermediates without a significant exposure potential?

When the indicator was developed, little robust information was available on the question whether substances are almost exclusively used as intermediates without a significant exposure potential. While it is known that some of the reference substances evaluated for the indicator are primarily used as chemical intermediates, this is not necessarily associated with a lack of significant exposure at the workplace or in the environment.

With the entry into force of REACH, additional information is available that facilitates the type of analysis required to answer the key question. For that purpose, an approach was developed that uses public information:

- from the dissemination database of registered substances (ECHA CHEM)([16]) of the European Chemicals Agency (ECHA), and
- from the PRODCOM database([17]), more specifically:
  - PRODCOM ANNUAL SOLD (NACE Rev. 2) (DS_066341) and
  - PRODCOM ANNUAL TOTAL (NACE Rev. 2) (DS_066342)

Public PRODCOM data were used in the development of this approach, since: a) they are more readily accessible, and b) a discussion of absolute figures was required for the evaluation, making it impossible to use the non-public, confidential PRODCOM data in this paper.

In a first step, all REACH registration types per substance were analysed for the substances

([16]) See: http://echa.europa.eu/web/guest/information-on-chemicals/registered-substances
([17]) See: http://ec.europa.eu/Eurostat/web/prodcom/data/database

evaluated within the indicator ‘Production of toxic chemicals’ (i.e. the reference substances selected for PRODCOM product groups, as identified by their CAS number).

The information disseminated on ECHA CHEM differentiates three types of registration, of which the following two are relevant in this context:

- Intermediate registration: applies to the use as an intermediate under strictly controlled conditions (SCC) according to REACH Articles 17 and 18;
- Full registration: applies to all other uses, but may also include uses as an intermediate under SCC

A substance may e.g. be registered with a full registration, with an intermediate registration or with both a full and intermediate registration. In addition, registrants may under certain circumstances submit individual dossiers rather than taking part in the regular joint submission. For example, a joint intermediate, an individual intermediate, a joint full and an individual full registration may exist for a given substance (four altogether), as observed for one of the substances in the indicator dataset.

9.3.2. Analysis

9.3.2.1. Registration types for reference substances evaluated within the Indicator

All 184 reference substances evaluated within the indicator with available CAS numbers were checked for the type of registration available on ECHA CHEM (i.e. disseminated substances, accessed: 20 August 2013) and the tonnage band for full registrations retrieved. Duplicate CAS number entries were removed (there are some PRODCOM product groups, for which the same reference substance was evaluated) to avoid a bias in the evaluation. Registration information was available for 139 of the substances/PRODCOM product groups evaluated for the indicator. The remainder may either not have been registered yet, has not been registered with the CAS number used in the evaluation, constituted duplicates or a CAS number was not available. A summary of the registration types of this dataset is shown in Table 10.

Table 10: Results of the evaluation using REACH registration types for reference substances in the dataset

Category	Number	Fraction
Total number of substances with registration	139	
FULL registration only	112	81 %
INTERMEDIATE registration only	3	2.2 %
FULL and INTERMEDIATE registration	24	17 %

These figures may be subject to change as more substances are registered and registration types are changed. While the detailed analyses performed in August-September 2013 and presented in the following sections could not be updated for the purposes of this paper, additional re-analyses were performed in September 2014 on selected issues discussed in more detail in the following sections. For the data presented in Table 10, such a re-analysis does not change the finding much (82 % full registrations only, 16 % full and intermediate registrations).

The results from this evaluation can be summarised as follows:

- The vast majority of substances (>80 %) evaluated has a full registration only.
- Only a very small fraction of substances is registered as intermediates only.
- The remaining substances have both a full and an intermediate registration.

Examples of references substances evaluated with their REACH registration types are given in Table 11 to give an idea of the substances and their respective registration types. For example, while the carcinogen buta-1,3-diene is usually cited as being used in closed systems as an intermediate for polymerisation and copolymerisation (ECB, 2002), this substance is only registered with full registrations (one joint and one individual registration)(18). In fact, the use descriptors in the joint full registration (1 000 000 - 10 000 000 tonnes per annum (tpa)) suggest an exposure potential to the environment (e.g. ERC(19) 8a and 8d for professional polymer processing) and at the workplace (e.g. PROC 7 (industrial spraying) and PROC 8a (transfers at non-dedicated facilities for many different uses)).

Table 11: Example of reference substances in the dataset with REACH registration types

Full registration only		**Full and intermediate registration**
Aniline	Ethene	Acetaldehyde
Buta-1,3-diene	Isoprene	Acetic anhydride
Carbon tetrachloride	Potassium hydroxide	Benzene
Chloroform	Sodium nitrate	Chromium trioxide
Diantimony trioxide	Sulphuric acid	Methyloxirane
Disodium carbonate	Vinyl chloride	**Intermediate registration only**
		Octan-2-ol

Note: some of the reference substances represent PRODCOM product groups (e.g. *isoprene* is evaluated for the PRODCOM entry 'Buta-1,3-diene and isoprene'); others are identical to the PRODCOM product group (e.g. *vinyl chloride* is a separate PRODCOM entry).

9.3.2.2. Indicator substances with full registrations only

A substance is generally registered with a full registration if one or more uses are not as an intermediate under strictly controlled conditions (SCC). Nonetheless, a full registration may also include the use as an SCC intermediate and registrants have chosen different approaches (i.e. integrating SCC intermediate uses in a full registration or submitting a separate intermediate registration) depending on a variety of considerations.

For substances with a full registration only, the extent to which it covers the use as an intermediate under SCC cannot be ascertained on the basis of publicly available data. There might therefore be cases where 99 % of the full registration tonnage band covers the use as an intermediate under SCC. However, there are some indications that substances with a full registration only might nonetheless represent cases with some potential for exposure (the ultimate criterion relevant here):

- Even if the full registration tonnage relates to a large extent to the use as an intermediate under SCC, a substantial tonnage for non-SCC intermediate uses remains for substances with high tonnages (that have the highest impact on the indicator). For example, if 99 % of the total tonnage of the full registration is used as an intermediate under SCC, 1 % remains for other uses with some potential for exposure. For a full registration tonnage band of
- 1 000 000 - 10 000 000 tpa, this equals 10 000 - 100 000 tpa, a considerable figure in absolute terms.
- An analysis of some substances with very high production tonnages indicates that strictly controlled conditions are generally not specifically mentioned in the use description. While this does not exclude such a use, the existence of individual examples (in which SCC is incorporated in the use description) appears to suggest that many intermediate uses are not under SCC.

([18]) When checked again in August 2014, only the joint full registration was left.
([19]) Environmental Release Categories according to ECHA (2010).

- The criticism by ECHA that some SCC claims may not be justified (see below) may lead to a considerable decline in such claims in the future.

9.3.2.3. Indicator substances with both a full registration and an intermediate registration

Substances for which both a full and an intermediate registration exist represent 17 % of the substances evaluated within the indicator (Table 10). The existence of both a full and an intermediate registration for a given substance generally suggests that the tonnage of the full registration covers uses other than the one as an intermediate under strictly controlled conditions. It may be anticipated that the tonnage of the full registration (for such a substance having both a full registration and a registration as an intermediate) is then lower compared to substances with a full registration only (i.e. no additional registration as an intermediate). A substantial fraction of the overall EU tonnage would then be 'hidden' in the registration as an intermediate (tonnage data for intermediate registrations are not published).

In order to further analyse this issue, indicator substances registered with a full registration only (n=112, see Table 10) and those registered with a full and an intermediate registration (n=24) were compared. This analysis is presented in more detail in the addendum below. It shows that substances registered both with a full and an intermediate registration under REACH have a tonnage band distribution similar to substances registered with a full registration only. This finding suggests that a large fraction of the tonnage is still assigned to the full registration, even if there is an intermediate registration for the same substance. As a consequence, there may be a considerable potential for exposure associated with uses other than the use as an intermediate under strictly controlled conditions.

It must be stressed that an intermediate registration relates to substances that are used as intermediates under strictly controlled conditions (REACH Articles 17 and 18). Some substances with a full registration only may also be primarily used as intermediates, either under strictly controlled conditions or not (also see the discussion above). Intermediates not handled under strictly controlled conditions may contribute substantially to exposure of workers and the environment. For example, the default worst-case release factors for the industrial use of intermediates (ERC 6a) of 5 % (to air) and 2 % (to wastewater) according to ECHA Guidance (ECHA, 2012a) suggest considerable releases to the environment under default (worst case) assumptions.

9.3.2.4. PRODCOM data for indicator substances with full and intermediate registrations

As is evident from the REACH registration data discussed above, the full registrations for these substances cover high tonnages and the data do not suggest that a high fraction of the tonnage is 'hidden' in the intermediate registration with confidential tonnages.

To further analyse this issue, the 24 indicator substances with both a full and an intermediate registration were compared in relation to the tonnage given for the REACH full registration and PRODCOM production figures (retrieved from the publicly available data for EU-27; data for 2010 were used, since most REACH registrations are from that year). The PRODCOM 'total production' (in contrast to the 'sold production') includes the produced amounts that are processed within the company (i.e. it potentially covers intermediate uses). Strictly controlled conditions may more easily be ascertained for a substance retained within the company compared to the amounts sold to other companies (when strictly controlled conditions must be confirmed along the entire supply chain). It can be assumed that the PRODCOM total production figure should be close to the sum of the REACH tonnage from the full registration (given as a tonnage band) and the REACH tonnage from intermediate registrations (which is not disclosed in the public ECHA CHEM database).

Again, details of this analysis are described in the addendum below. In summary, several findings emerge from this evaluation:

- The PRODCOM total production tonnages are generally in agreement with full REACH registration tonnages, since they are higher than the maximum or are between the minimum and the maximum full REACH registration tonnage.

- For eight substances, PRODCOM total production is higher than the maximum of the full REACH, suggesting that a substantial fraction of the amount produced may need to be assigned to the REACH registration as an intermediate. PRODCOM total production for these substances, however, is low (maximum about 1 000 000 tpa) and the impact on the indicator is therefore also low.
- The largest group of 13 substances has PRODCOM total production tonnages between the minimum and maximum of the full REACH registration. As a consequence of the wide range between minimum and maximum, no definitive conclusions can be drawn.
- Overall, the analysis of full registration tonnages and the comparison with PRODCOM data for substances with both a full and an intermediate REACH registrations does not support the notion that most of the substances contributing to the indicator are primarily used as intermediates under strictly controlled conditions with little potential for exposure.

9.3.2.5. Indicator substances with registrations as intermediates only

Finally, the PRODCOM total production data for the three indicator substances registered as intermediates only (see Table 10) were retrieved. Their PRODCOM total production volumes range between 206 370 and 1 199 521 tpa. Therefore, these three substances do not have a large impact on the indicators discussed in this paper.

In the context of intermediate registrations in general, the potential impact of the criticism by ECHA already mentioned above is important. The Agency questioned the validity of the definition of intermediates and/or that strictly controlled conditions can be confirmed for more than 2 300 dossiers from intermediate registrations([20]). According to this news alert, some of these dossiers are being updated into full registrations. When checking the substances with both full and intermediate registrations again in September 2014, we observed that this was the case for 2/23 (8.7 %) of the substances, indicating that such an update is taking place. Of the three substances registered as intermediates only, all three still had only an intermediate registration when re-analysed in September 2014.

9.3.2.6. Very high production volume substances

As a last step, an additional analysis approached the questioned from the other end. Since the tonnage has a large impact on the indicator, public PRODCOM total production figures were extracted and the results for entries/substances evaluated were sorted in descending order. Note that some high production PRODCOM entries are exempted from registration and evaluation under REACH (e.g. *oxygen* and *hydrogen*). Some others were too broad to be evaluated for the indicator or were not evaluated for some other reason. The data in Table 12 show the result of this analysis for substances with a PRODCOM total production above 4 000 000 tpa (arbitrarily chosen). The data indicate that among the very high production PRODCOM entries, the vast majority (13/16) of substances is registered with a full registration only, corresponding to 81 %, a figure that is identical to the entire dataset of reference substances (see Table 10). Since none of these very high production chemicals is registered with an intermediate registration only, the figure for substances registered with both a full and an intermediate registration of (3/16 =) 19 % is slightly higher than in the entire dataset.

([20]) http://echa.europa.eu/view-article/-/journal_content/title/echa-receives-updates-for-intermediate-dossiers-and-announces-further-follow-up-actions

Table 12: High production PRODCOM entries evaluated for the indicator and REACH registration type

PRODCOM entry (PRCCODE)*	PRODCOM total production (tpa)	Registration type
Unsaturated acyclic hydrocarbons; ethylene	19 538 120	FULL only
Sulphuric acid	15 451 515	FULL only
Anhydrous ammonia	12 931 332	FULL & INTERMEDIATE
Sodium hydroxide in aqueous solution (soda lye or liquid soda)	9 086 567	FULL only
Chlorine	8 885 007	FULL & INTERMEDIATE
Disodium carbonate	7 724 407	FULL only
Nitric acid; sulphonitric acids	7 566 829	FULL only
Benzene	6 505 856	FULL & INTERMEDIATE
Vinyl chloride (chloroethylene)	6 031 666	FULL only
1.2-Dichloroethane (ethylene dichloride)	5 277 897	FULL only
Hydrogen chloride (hydrochloric acid)	5 110 677	FULL only
Styrene	4 981 758	FULL only
Calcium carbonate	4 793 204	FULL only
Ammonium nitrate (excluding in tablets or similar forms or in packages of a weight of <= 10 kg)	4 495 742	FULL only
Ethylbenzene	4 346 398	FULL only
Naphthalene and other aromatic hydrocarbon mixtures (excluding benzole, toluole, xylole)	4 019 958	FULL only

* If the PRODCOM entry does not unambiguously identify a specific substance, the substance evaluated for the indicator 'Production of toxic chemicals' is set in **bold**

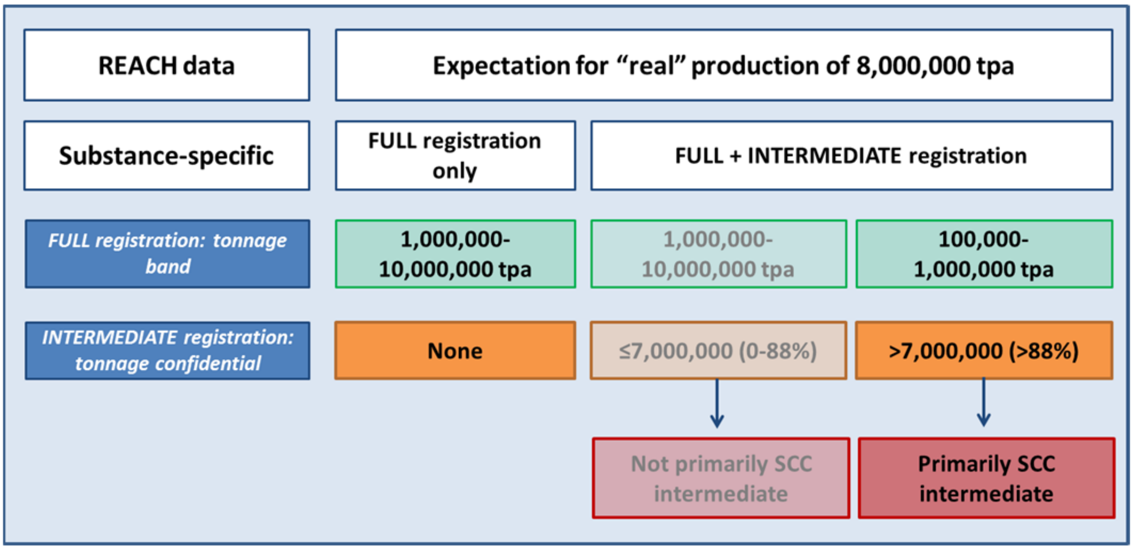
In agreement with the high PRODCOM total production, these substances are almost exclusively registered under REACH at the higher tonnage bands (10 000 000 - 100 000 000 tpa (n=7); 1 000 000 - 10 000 000 tpa (n=8)). When re-analysed in September 2014, two of the substances with a full registration only in August 2013 had an additional intermediate registration. As already discussed above, *anhydrous ammonia* 'lost' its intermediate registration and has only a full registration. While the number of the substances with a full registration only is therefore reduced from 13 to 12, they still represent the majority of substances in this set (75 %).

Overall, these data corroborate the findings of the previous evaluations and clearly demonstrate that those substances with a very high PRODCOM total production - and therefore a high impact on the indicator - are most probably not primarily handled under strictly controlled conditions. As discussed above, there may be cases among these substances where intermediate uses under strictly controlled conditions are included in the full registration. However, the fact that a full registration exists for these substance is clear evidence that uses other than SCC intermediate uses also exist. Even if such uses account for only a small fraction (e.g. 0.1 %, i.e. 99.9 % SCC intermediate uses) a substantial tonnage (≥ 4 000 tpa in this example for the substance shown in the table above) would not be handled under strictly controlled conditions and could thus contribute to the exposure of humans.

9.3.3. Addendum: Comparison of indicator substances registered with a full registration and those registered with a full and an intermediate registration

For substances with both full and intermediate registrations, one would expect to see a lower tonnage band for the full registration compared to substances with a full registration only if a substantial fraction is used as an intermediate under strictly controlled conditions (i.e. registered with a high (confidential) tonnage in the intermediate registration). The rationale for this assumption is shown in Figure 18 for an assumed 'real' production (in fact: manufacture and imports) of a substance of 8 000 000 tpa. If such a substance is only registered with a full registration, the tonnage band should be 1 000 000-10 000 000 tpa. If this substance is registered with both a full and an intermediate registration, the tonnage band of the full registration may be the same. The fraction to be assigned to the use as an intermediate under strictly controlled conditions may then range from zero to 88 %. If, however, the substance is primarily used as an intermediate under strictly controlled conditions, a large fraction of the overall tonnage should be 'hidden' in the intermediate registration. As a consequence, the tonnage band of the full registration should be lower (100 000-1 000 000 tpa in this example).

Figure 18: Tonnage band discrimination of substances with a full registration and substances with both a full and an intermediate registration



It should be noted that the figure serves for illustration purposes only and no 'cut-off' (e.g. the 88 % used in the example) should be derived.

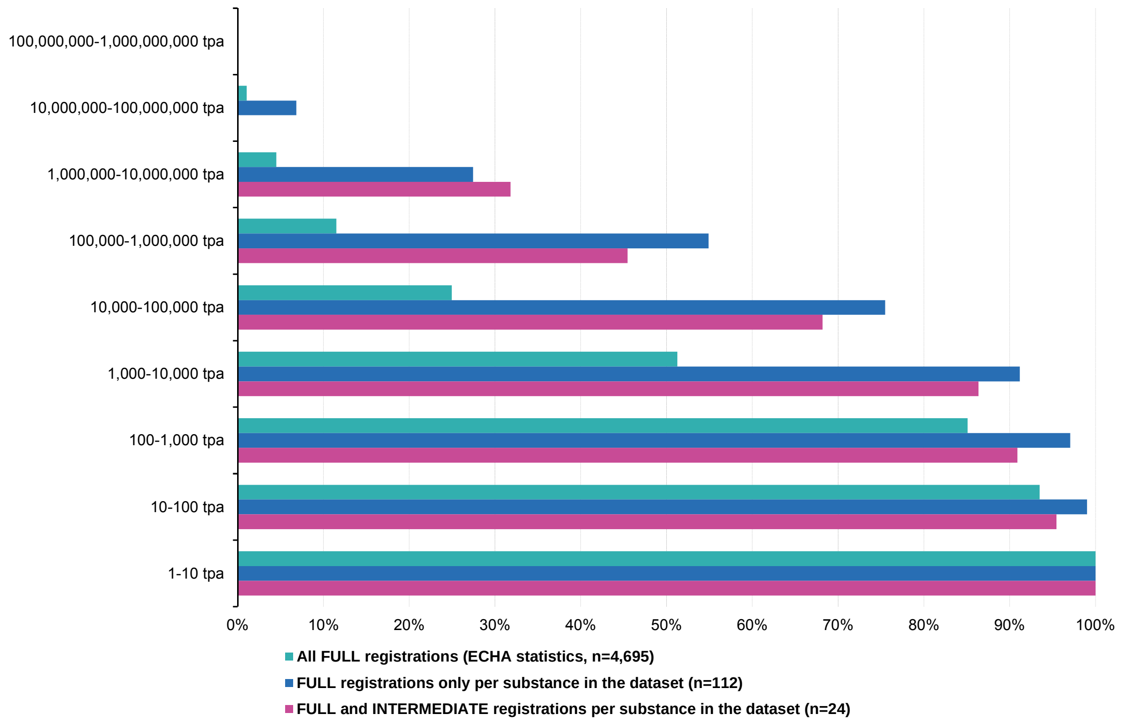
For the 136 (112 + 24) substances with full registrations, discrete tonnage band information was available for 123 (90 %) substances, with the remainder only having lower tonnages (e.g. 10 000 + tpa) assigned, since confidentiality was claimed by registrants. These were assigned to the lowest meaningful tonnage band (in this example: 10 000 - 100 000 tpa). The data for the reference substances in the dataset were compared with data for all full registrations according to ECHA statistics([21]).

Reference substances in the dataset evaluated for the indicator are registered with full registrations at high tonnages. For example, almost 60 % of the reference substances have full registrations at 100 000 tpa or above, while this figure is only 11.5 % for all substances registered with full registrations according to ECHA statistics. This illustrates the fact that the indicator is based on substances with high production volumes, since substances with low tonnages are generally not included in PRODCOM as discrete entities. Such substances are expected to be covered broad

([21]) http://echa.europa.eu/information-on-chemicals/registration-statistics, accessed: August 2013

PRODCOM entries, such as ‘Saturated acyclic hydrocarbons’ or ‘Unsaturated chlorinated derivatives of acyclic hydrocarbons (excluding vinyl chloride, trichloroethylene, tetrachloroethylene)’). Note that the percentage of higher tonnage bands in the evaluation of all full registrations (according to ECHA statistics) will certainly decrease further in the future, as the lower tonnage bands are registered.

Figure 19: Tonnage band information for reference substances in the dataset compared to all substances registered: cumulative percentage of substances



Even if a substance is registered both with a full and an intermediate registration under REACH, the tonnage for the full registration is high and the distribution is similar to substances registered with a full registration only. Both sets have a substantially higher fraction of substances in the higher tonnage bands when compared with all full registrations. This finding is not unexpected since the indicators substances largely represent substances produced at high tonnages. The anticipated shift towards lower full registration tonnages for substances with both a full and an intermediate registration (compared to those with a full registration only, see Figure 18) is not evident in Figure 19 for the reference substances in the dataset. There are some differences between the figures for the reference substances with a full registration only and those with both a full and an intermediate registration. However, the differences are small and are clearly less pronounced than the difference between these two sets of substances and the data for all full registrations.

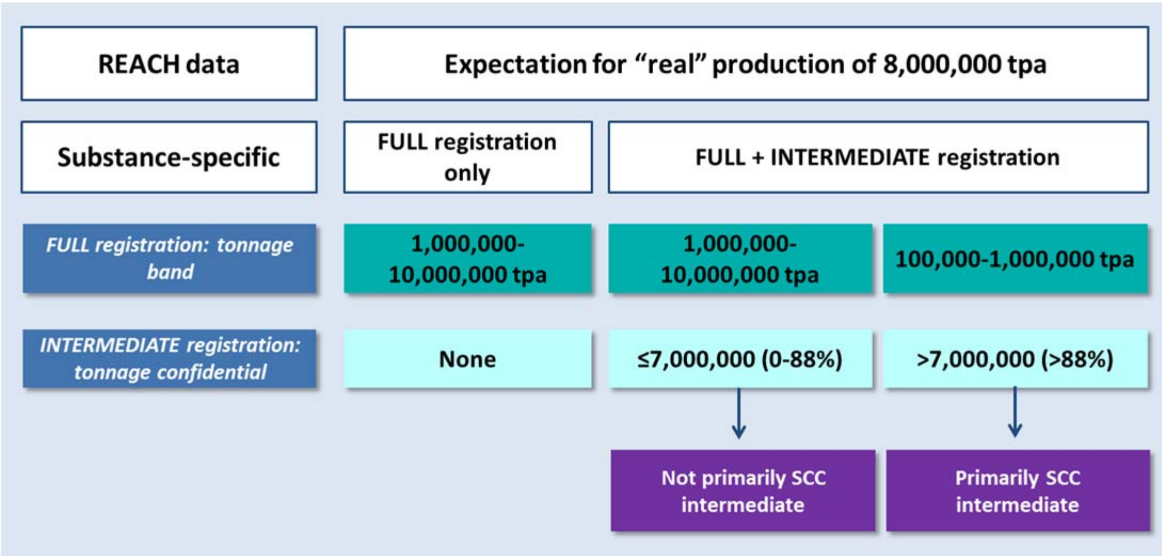
This analysis suggests that indicator substances are not primarily intermediates handled under strictly controlled conditions (i.e. without a significant exposure potential). However, it suffers from the unclear picture in relation to substances with a full registration only that is discussed above.

In this context, it must again be stressed that an intermediate registration relates to substances that are used as intermediates under strictly controlled conditions (REACH Articles 17 and 18). Some substances with a full registration only may also be primarily used as intermediates, either under strictly controlled conditions or not (also see the discussion above). Intermediates not handled under strictly controlled conditions may contribute substantially to exposure of workers and the environment. For example, the release factors for industrial use of intermediates (ERC 6a) of 5 % (to air) and 2 % (to wastewater) according to ECHA Guidance (ECHA, 2012a) suggest considerable releases to the environment under default (worst case) assumptions.

Substances for which both a full and an intermediate registration exist represent 17 % of the substances evaluated within the indicator (Table 10). As is evident from the REACH registration data alone, the full registrations for these substances cover high tonnages and the data do not suggest that a high fraction of the tonnage is 'hidden' in the intermediate registration with confidential tonnages (see Figure 19 and the discussion above).

To further analyse this issue, the 24 indicator substances with both a full and an intermediate registration were compared in relation to the tonnage given for the REACH full registration and PRODCOM production figures (retrieved from the publicly available data for EU-27; data for 2010 were used, since most REACH registrations are from that year). The PRODCOM 'total production' (in contrast to the 'sold production') includes the produced amounts that are processed within the company (i.e. it potentially covers intermediate uses). Strictly controlled conditions may more easily be ascertained for a substance retained within the company compared to the amounts sold to other companies (when strictly controlled conditions must be confirmed along the entire supply chain). It can be assumed that the PRODCOM total production figure should be close to the sum of the REACH tonnage from the full registration (given as a tonnage band) and the REACH tonnage from intermediate registrations (which is not disclosed in the public ECHA CHEM database). The relationship between the different data is shown in Figure 20.

Figure 20: **Comparison of REACH data and PRODCOM data for production figures**



It is evident that the (unknown) tonnage for the REACH intermediate registration may be approximated from the PRODCOM total production minus the tonnage of the REACH full registration. Since the latter is only given as a tonnage band, with minimum and maximum differing by a factor of 10, such an estimate is very rough.

The calculations involved are presented in Box 1 using *chlorosulphoric acid* as an example.

EXAMPLE FOR THE COMPARISON REACH – PRODCOM

The calculations performed are illustrated using the example of '*chlorosulphoric acid*' (substance no. 4 in Table 13). The PRODCOM total production is 14 000 tpa, while the full REACH registration is for the 100-1 000 tpa band. According to the disseminated dossier of the full registration, the substance is used industrially in polymer preparations and compounds (PC 32), in washing and cleaning products (PC 35) as well as an intermediate (PC 19), the latter possibly not under SCC (since this can be expected to be covered by the intermediate registrations). Two intermediate REACH registrations exists (one joint and one individual submission) and the tonnage for these intermediate registrations was calculated to be at least (14 000 tpa – 1 000 tpa =) 13 000 tpa or 93 % of the PRODCOM total production. This figure is based on the maximum of the full registration (1 000 tpa) and increases to (14 000 tpa - 100 tpa =) 13 900 tpa or 99 % of the PRODCOM total production, if the minimum of the full registration is used (see column 'calculated % intermediate' in the following table). In this example, the substance appears to be primarily used as an SCC intermediate.

Table 13 shows the results for such an approximation for the substances with both full and intermediate REACH registrations (see Table 10, n=23, since PRODCOM data could not be retrieved for one substance at the time of analysis).

Data from the PRODCOM SOLD database were included in the evaluation in order to get an idea on import and export figures, which are not included in PRODCOM TOTAL. Note that for the example of *chlorosulphuric acid*, imports and exports are roughly equal. The PRODCOM SOLD tonnage, however, is only 50 % of the PRODCOM TOTAL tonnage. This figure suggests substantial use within the company (potentially as an intermediate under strictly controlled conditions; see discussion above).

As a first finding of this analysis, the data in Table 13 show that (with the exception of chloromethane and methanol discussed in detail below) the figures from REACH registrations and from PRODCOM agree very well. While PRODCOM 'total production' is higher than the REACH full registration tonnage for substances 1-8, this can be explained by the tonnage 'hidden' in the intermediate registration (in fact, this is the rationale of the analysis presented here). For substances 9-21, the PRODCOM 'total production' is within the REACH full registration. While the tonnage of the intermediate registration remains an uncertainty, the agreement between these very different data sources is remarkable.

Table 13: Comparison of tonnage data in REACH registrations and PRODCOM to delineate uses for substances with both full and intermediate REACH registrations

	Reference substance in the dataset	Tonnage of full REACH registration [tpa]		PRODCOM TOTAL		Calculated % intermediate*		PRODCOM SOLD			
		Min	Max	Production	represents	Min	Max	Production	Import	Export	Consumption
1	Acetaldehyde	10	100	150 419	Substance	100 %	100 %	66 766	3 791	32	70 525
2	Diethylamine	1 000	10 000**	442 347	Group	98 %	100 %	119 198	8 152	5 644	121 706
3	Dibutyl phthalate	1 000	10 000	211 232	Group	95 %	100 %	213 097	5 804	76 087	142 814
4	Chlorosulphuric acid	100	1 000	14 000	Substance	93 %	99 %	7 000	8 036	7 000	8 036
5	Ethylenediamine	10 000	100 000**	1 028 487	Group	90 %	99 %	752 729	33 264	73 530	712 463
6	Nickel dihydroxide	1 000	10 000	62 089	Group	84 %	98 %	18 867	21 983	2 846	38 004
7	Chromium trioxide	10 000	100 000	350 147	Group	71 %	97 %	230 557	98 448	39 313	289 692
8	Allyl alcohol	10 000	100 000	214 745	Group	53 %	95 %	28 964	12 442	7 945	33 461
9	Chlorine	1 000 000	10 000 000	8 885 007	Substance	0 %	89 %	4 710 012	8 926	31 900	4 687 038
10	Benzoyl chloride	10 000	100 000	80 000	Group	0 %	88 %	25 538	4 632	12 150	18 020
11	Benzene	1 000 000	10 000 000	6 505 856	Substance	0 %	85 %	5 071 474	652 117	104 023	5 619 568
12	Formaldehyde	1 000 000	10 000 000**	3 479 917	Substance	0 %	71 %	1 293 109	11 612	29 132	1 275 589
13	Butanone	100 000	1 000 000	316 703	Substance	0 %	68 %	222 461	6 299	59 175	169 585
14	Methyloxirane	1 000 000	10 000 000**	2 512 383	Substance	0 %	60 %	1 847 808	61 433	73 007	1 836 234
15	Ethylene oxide	1 000 000	10 000 000**	2 372 821	Substance	0 %	58 %	911 396	943	12 570	899 769
16	Bis(2-ethylhexyl) phthalate	100 000	1 000 000	211 232	Group	0 %	53 %	213 097	5 804	76 087	142 814
17	Maleic anhydride	100 000	1 000 000	207 035	Substance	0 %	52 %	89 176	44 875	3 429	130 622
18	Sulphur	1 000 000	10 000 000	1 950 630	Substance	0 %	49 %	1 951 800	1 626	14 021	1 939 405

	Reference substance in the dataset	Tonnage of full REACH registration [tpa]		PRODCOM TOTAL		Calculated % intermediate*		PRODCOM SOLD			
		Min	Max	Production	represents	Min	Max	Production	Import	Export	Consumption
19	Acetic anhydride	100 000	1 000 000	183 255	Substance	0 %	45 %	140 000	133 220	12 567	260 653
20	Acrylic acid	1 000 000	10 000 000	1 717 325	Group	0 %	42 %	874 010	32 177	63 864	842 323
21	Ammonia, anhydrous	10 000 000	100 000 000	12 931 332	Substance	0 %	23 %	3 645 786	-	-	3 645 786
22	Chloromethane	1 000 000	10 000 000	372 759	Group			265 240	3 338	3 835	264 743
23	Methanol	10 000 000	100 000 000	1 801 466	Substance			1 258 890	5 675 397	155 957	6 778 330

* Calculated percent intermediate registration tonnage: (PRODCOM TOTAL Production - minimum (maximum) tonnage of full REACH registration) / PRODCOM TOTAL Production; values presented in tonnes per annum (tpa) and percent of the PRODCOM TOTAL production;

** full registration tonnage given as minimum (e.g. 1 000+) and not as band; maximum derived by multiplying the minimum by a factor of 10.

While such calculations obviously suffer from the broad range of tonnages assigned to full REACH registrations and the limitations of the published PRODCOM data (some being e.g. estimates), several findings emerge from this evaluation:

- In general, the PRODCOM total production tonnages are in agreement with full REACH registration tonnages, since they are higher than the maximum (substances 1-8; potentially indicating uses as intermediates under strictly controlled conditions; see below) or are between the minimum and the maximum full REACH registration tonnage (substances 9-21; also see discussion above). Note that - with very few exceptions - the same is basically also true for consumption figures. Only 2/23 substances show a pattern where REACH full registration and PRODCOM tonnages are in disagreement (see discussion below).
- For substances 1-8 in Table 13, PRODCOM total production is higher than the maximum of the full REACH registration by a factor of 2 (allyl alcohol) to 1,500 (acetaldehyde), suggesting that more than half (allyl alcohol, chromium trioxide) or almost all (acetaldehyde and some other substances) of the amount produced may need to be assigned to the intermediate REACH registration. Note that PRODCOM total production is taken here as the ‘real’ production as described in Figure 18and the full registration tonnages are indeed low (see discussion above).
- However, the conclusion that these eight substances are primarily (at least >50 %) used as intermediates under strictly controlled conditions should be interpreted with the following issues in mind:
    - The PRODCOM total production volume refers to group entries for 6/8 substances in the first group, while the full REACH registration tonnage refers to individual substances selected to be representative of the PRODCOM product group. In some cases, other substances covered by the same product group may be responsible for the high PRODCOM total production. This is most evident for *dibutyl phthalate* (substance no. 3), which is covered by the same PRODCOM product group as *bis(2-ethylhexyl) phthalate* (substance no. 16), the latter having a much higher full REACH registration. As another example, *ethylenediamine* is covered by the PRODCOM product group *hexamethylenediamine and its salts; ethylenediamine and its salts* and *hexamethylenediamine* is only registered with a full REACH registration (100 000-1 000 000 tpa), the upper end approaching the PRODCOM total production.
    - For two of these eight substances (*diethylamine* and *ethylenediamine*), the full REACH registration tonnage was given as a lower end value for confidentiality reasons. The maximum was derived as 10-times the minimum, but may in fact be higher (also see discussion for *ethylenediamine* above).

Nonetheless, the two substances evaluated that are directly represented in PRODCOM (*acetaldehyde* and *chlorosulphuric acid*) are clearly examples where the production (according to PRODCOM total) is much higher than the tonnage band of the full REACH registration, suggesting that these substances are primarily used as intermediates under strictly controlled conditions. The same may also apply to *allyl alcohol*, since the total production is more than 6-times higher than the sold production (or consumption), implying that a substantial fraction remains within the company. However, allyl alcohol represents a PRODCOM product group with the associated problems discussed above.

Overall, PRODCOM total production tonnages for all eight substances in this group are low (compared e.g. to substances 9-21). The impact of these substances on the indicator is therefore low.

- The largest group of 13 substances has PRODCOM total production tonnages between the minimum and maximum of the full REACH registration. As a consequence of the wide range between minimum and maximum, no definitive conclusions can be drawn. Thus, very small fractions of the substance produced may be used as an intermediate under strictly controlled conditions (indicated by ‘0 %’ in the table; the existence of an intermediate REACH registration, however, indicates that some fraction of the PRODCOM total production will be used as an SCC intermediate). The opposite may, however, just as well be true, i.e. the intermediate registration may account for up to 89 % (chlorine) of the PRODCOM total production. In addition, some of the substances evaluated represent PRODCOM product groups (see discussion above). For these reasons, the following discussion focusses on substances directly representing PRODCOM entries (i.e. not group entries representing two or more substances) produced at very high tonnages, since these will have a high impact within the indicator system:

- ***Ammonia, anhydrous***: the PRODCOM total production is close to the lower end of the full REACH registration, implying that only a small fraction (up to 23 %) may be assigned to the intermediate REACH registration. While the PRODCOM sold production is much lower than the PRODCOM total production (suggested above to be indicative of intermediate uses, potentially under strictly controlled conditions), the vast array of different manufacturing and use scenarios (both industrial and professional) given in the disseminated dossier of the full registration support the notion of a high fraction of uses not under strictly controlled conditions. In addition, the intermediate registration for this substance contains many use scenarios with descriptors (e.g. PROC 5, ERC 4), which are not compliant with an intermediate registration according to ECHA([22]). The intermediate registration for *ammonia, anhydrous* may thus be one of the many intermediate registrations, for which ECHA questioned the fulfilment of the definition of intermediates and/or the use being under strictly controlled conditions and asked registrants to carefully review and update registration dossiers([23]). In agreement with this suggestion, the intermediate registration retrieved in August 2013 was no longer available on ECHA CHEM, when checked again in September 2014. Only two full registrations remained, one joint submission with the high tonnage reported in Table 13 (10 000 000-100 000 000 tpa) and one individual submission with a substantially lower tonnage band (100-1 000 tpa).
- ***Chlorine***: The PRODCOM total production is considerably higher than the minimum of the full REACH registration, implying that a large fraction (up to 89 %) may be assigned to the intermediate REACH registration. This is also suggested by the fact that PRODCOM sold production is only 53 % of PRODCOM total production. There is no doubt that chlorine is primarily used as an intermediate; the question is whether these intermediate uses are under strictly controlled conditions (required for an intermediate registration) or not. In this context, it is important to note that the full REACH registration for chlorine covers several uses as an intermediate and only few of these are described as being under strictly controlled conditions. In fact, the 2007 EU Risk Assessment Report indicates that occupational exposure during use as an intermediate occurs (typical: 0.216-0.25; reasonable worst case: 0.501-0.705 mg/m^3, largely derived from measured data). The reasonable worst case (i.e. 90th percentile) exposure values are only slightly below the long-term DNEL derived for workers in the REACH registration dossier (0.75 mg/m^3).
- ***Benzene***: This substance shows a pattern similar to chlorine in that PRODCOM total production is considerably higher than the minimum of the full REACH registration. In contrast to chlorine, however, PRODCOM sold production is 78 % of PRODCOM total production, implying that a large fraction is not used within the company and may be less likely to be handled under strictly controlled conditions. The EU Risk Assessment Report noted that ‘occupational exposure to benzene occurs mainly in the production of benzene and its further processing as a chemical intermediate as well as in the refinery and distribution of gasoline’ and derived a reasonable worst case concentration from measured data (95th percentile) of 3.5 mg/m^3 for manufacture and processing in the large scale chemical industry (not differentiated). Note that such an exposure level is slightly above the EU ‘Binding Occupational Exposure Limit Value’ of 3.25 mg/m^3 according to Council Directive 2004/37/EC([24]). It is assumed to be associated with a relevant cancer risk

([22]) See http://echa.europa.eu/documents/10162/13583/intermediate_status_scc_background_note_en.pdf
([23]) See http://echa.europa.eu/view-article/-/journal_content/0d1a14fe-9c63-4807-a3de-380c0dbffdf5
([24]) Council Directive 2004/37/EC of the European Parliament and of the council of 29 April 2004 on the protection of workers from the risks related to exposure to carcinogens or mutagens at work.

according to the German exposure-risk relationship values(25).

These examples show that the use as an intermediate may be associated with substantial occupational exposure.

- The last two substances in Table 13 deserve special attention since the PRODCOM total production is lower than the minimum of the full REACH registration. In the case of *methanol* the high imports (which have to be contained in the registration tonnage) partly explain this deviation, but even the sum of PRODCOM total production and imports is below the minimum of the full REACH registration. Checking data for the years 2009, 2011 and 2012 does not resolve this issue. One possible explanation is that registrants have chosen tonnages representing plant capacities and projected imports rather than actual production/import figures. Similar to *anhydrous ammonia*, the intermediate registration retrieved in August 2013 for *methanol* was no longer available on ECHA CHEM in September 2014, suggesting that intermediate use under strictly controlled conditions was reviewed and the dossiers updated(26). For *chloromethane*, the deviation between PRODCOM total production and minimum tonnage of the full REACH registration cannot be solved and, again, the registration tonnage may refer to plant capacities rather than actual production. In support of this, based on 1997 production tonnages of 630 000 (USA) and 180 000 tpa (Japan)(27) and the classification of the substance as a suspected carcinogen, the PRODCOM figures for EU-27 in 2010 (372 759 tpa total production) appear to be more realistic than the minimum tonnage of the full REACH registration (1 000 000 tpa). In this case, the PRODCOM entry only refers to two substances (chloromethane and chloroethane) and the full REACH registration for chloroethane (1 000-10 000 tpa) is much lower than for chloromethane (1 000 000 - 10 000 000), see Table 9.
- In summary, it is difficult to impossible to derive figures for the intermediate REACH registration for many of the substances registered with both a full and an intermediate registration. However, the following conclusions can be drawn:
  - There are some individual examples (*acetaldehyde, chlorosulphuric acid*), for which a large fraction of the PRODCOM total production most probably relates to the use as an intermediate under strictly controlled conditions.
  - For many other substances, even the minimum tonnage of the full REACH registration is high (≥1 000 000 tpa for 8/13 substances) and accounts for a substantial fraction of the PRODCOM total production (e.g. 11-77 % for substances 9-21). Although this tonnage may also include SCC intermediate uses, PRODCOM SOLD and calculated consumption figures ≥1 000 000 tpa for six of these eight substances suggest that use of these may be associated with a potential exposure (even if 99 % is assigned to SCC-intermediate uses, the tonnage for other uses is still comparatively high (≥10 000 tpa).
  - However, full REACH registration tonnages may sometimes be too high (e.g. when they reflect plant capacities rather than actual production figures), thus overestimating the fraction of the PRODCOM total production that is related to potential exposure. On the other hand, many substances were evaluated as a reference for a wider PRODCOM product group. The PRODCOM total production for the individual substance is therefore lower, decreasing the fraction of the PRODCOM total production assigned to intermediate uses under strictly controlled conditions.

Overall, the analysis of full registration tonnages and the comparison with PRODCOM data for substances with both a full and an intermediate REACH registrations does not support the notion that most of the substances contributing to the indicator are primarily used as intermediates under strictly controlled conditions with little potential for exposure.

(25) For a detailed documentation of the respective values (in German), see: http://www.baua.de/de/Themen-von-A-Z/Gefahrstoffe/TRGS/Begruendungen-910.html

(26) Anhydrous *ammonia* and methanol are the only two substances of those presented in Table 13 for which the intermediate registration retrieved in August 2013 was no longer available in September 2014.

(27) Both figures according to OECD SIDS: http://webnet.oecd.org/Hpv/UI/handler.axd?id=dd47eb96-57df-4a0a-afcc-3c1453ac2b3c

9.4. Annex 4: Toxicity classes of indicator substances

The following lists contain the PRODCOM entry as well as the CAS number of the substance evaluated for each PRODCOM entry (n=184) differentiated by toxicity class (according to H-statements) for the indicator 'Production of toxic chemicals'. Some substances are evaluated for more than one PRODCOM entry.

Table 14: Summary of the assignment to toxic impact classes per substance evaluated

Class A (n=34)

PRODCOM entry	CAS number of substance evaluated
Sulphur trioxide (sulphuric anhydride); diarsenic trioxide	1327-53-3
Chromium trioxide	1333-82-0
Lead monoxide (litharge, massicot)	1317-36-8
Red lead and orange lead	1314-41-6
Lead oxides, n.e.c.	68411-78-9
Nickel oxides and hydroxides	12054-48-7
Pigments and preparations based on chromium compounds	7758-97-6
Pigments and preparations based on cadmium compounds	10124-36-4; 1306-19-0
Mercury	7439-97-6
Oxides of boron; boric acids, inorganic acids other than hydrogen fluoride	10043-35-3
Hydrazine and hydroxylamine and their inorganic salts	302-01-2
Lead carbonate	598-63-0
Chromates of zinc or of lead	Index no. 024-007-00-3
Sodium, potassium dichromates and other chromates and peroxochromates	7789-00-6
Disodium tetraborates and other borates (excl. peroxoborates (perborates))	1330-43-4
Peroxoborates (perborates)	7632-04-4
Buta-1,3-diene	106-99-0
Unsaturated acyclic hydrocarbons; Isoprene	78-79-5
Benzene	71-43-2
1,2-Dichloroethane (ethylene dichloride)	107-06-2
Vinyl chloride (chloroethylene)	75-01-4
Trichloroethylene	79-01-6
Hexachlorobenzene and DDT (1,1,1-trichloro-2, 2-bis(p-chlorophenyl)ethane)	118-74-1
Cobalt acetates	6147-53-1
Dibutylorthophthalate	84-74-2
Dioctyl orthophthalates	117-81-7
Acrylonitrile	107-13-1
Oxirane (ethylene oxide)	75-21-8
Methyloxirane (propylene oxide)	75-56-9
Wood tar; wood tar oils; wood creosote; wood naphtha etc.	61789-60-4

PRODCOM entry	CAS number of substance evaluated
Phenols	91079-47-9; 84988-93-2
Creosote oils	90640-84-9
Other oils and oil products n.e.c.	91995-16-3
Pitch and pitch coke,obtained from coal tar or from other mineral tars	94114-13-3

Class B (n=30)

PRODCOM entry	CAS number of substance evaluated
Sulphur trioxide (sulphuric anhydride); diarsenic trioxide	1327-53-3
Cobalt oxides and hydroxides; commercial cobalt oxides	1307-96-6
Vanadium oxides and hydroxides	1314-62-1
Molybdenum oxides and hydroxides	1313-27-5
Antimony oxides	1309-64-4
Carbon disulphide	75-15-0
Peroxosulphates (persulphates)	7727-54-0
Toluene	108-88-3
Naphthalene, anthracene	91-20-3
Chloromethane (methyl chloride) and chloroethane (ethyl chloride)	74-87-3
Dichloromethane (methylene chloride)	75-09-2
Chloroform (trichloromethane)	67-66-3
Carbon tetrachloride	56-23-5
Tetrachloroethylene (perchloroethylene)	127-18-4
Unsaturated chlorinated derivatives of acyclic hydrocarbons n.e.c.	542-75-6
1, 2, 3, 4, 5, 6-Hexachlorocyclohexane	319-84-6; 319-85-7
Phenol (hydroxybenzene) and its salts	108-95-2
4,4-isopropylidenediphenol (bisphenol A, diphenylolpropane) and salts	80-05-7
Vinyl acetate	108-05-4
Benzoyl peroxide and benzoyl chloride	98-88-4
Maleic anhydride	108-31-6
Phthalic anhydride	85-44-9
Ethylenediamine and its salts	107-15-3
Aniline and its salts	62-53-3
Methanal (formaldehyde)	50-00-0
Ethanal (acetaldehyde)	75-07-0
Paraformaldehyde	30525-89-4
Gum, wood or sulphate turpentine oils,pine oil and other alike	8006-64-2
Rosin and resin acids, and derivatives; rosin spirit and oils; run gums	73138-82-6
Naphthalene and other aromatic hydrocarbon mixtures	91-20-3; 84650-04-4

Class C (n=30)

PRODCOM entry	CAS number of substance evaluated
Nitrogen oxides	10102-44-0
Manganese oxides (excl. manganese dioxide)	1317-35-7
Iodine	7553-56-2
Fluorine	7782-41-4
Bromine	7726-95-6
Phosphorus	12185-10-3
Chlorides and chloride oxides of phosphorus	10025-87-3; 10026-13-8
Rare-earth metals, scandium and yttrium	7440-65-5
Hydrogen chloride (hydrochloric acid)	7647-01-0
Chlorosulphuric acid	7790-94-5
Sulphuric acid	7664-93-9
Oleum	8014-95-7
Diphosphorus pentaoxide	1314-56-3
Hydrogen fluoride (hydrofluoric acid)	7664-39-3
Sodium hydroxide (caustic soda), solid	1310-73-2
Sodium hydroxide in aqueous solution (soda lye or liquid soda)	1310-73-2
Potassium hydroxide (caustic potash), solid	1310-58-3
Potassium hydroxide in an aqueous solution	1310-58-3
Peroxides of sodium or potassium	1313-60-6
Other salts of oxometallic and peroxometallic acids, n.e.c.	1313-60-6
Cyanides, cyanide oxides and complex cyanides	74-90-8
Hydrogen peroxide	7722-84-1
Phosphides excluding ferrophosphorous	20859-73-8; 1305-99-3; 12057-74-8
Styrene	100-42-5
Formic acid	64-18-6
Acetic acid	64-19-7
Acrylic acid and its salts and other monocarboxylic acid	79-10-7
Methacrylic acid and its salts	79-41-4
Diethylamine and salts	109-89-7
Nitric acid; sulphonitric acids	7697-37-2; 51602-38-1

Class D (n=49)

PRODCOM entry	CAS number of substance evaluated
Zinc oxide; zinc peroxide	1314-13-2
Titanium oxides	13463-67-7

PRODCOM entry	CAS number of substance evaluated
Manganese dioxide	1313-13-9
Iron oxides and hydroxides containing >= 70% iron(III) oxide	1309-37-1
Earth colours containing >= 70% iron(III) oxide	1309-37-1
Lithium oxide and hydroxide	1310-65-2
Pigments and preparations based on titanium dioxide, >= 80% of titanium dioxide	13463-67-7
Pigments and preparations based on titanium dioxide, other	13463-67-7
Chlorine	7782-50-5
Arsenic	7440-38-2
Selenium	7782-49-2
Sodium	7440-23-5
Alkali metals (excl. sodium)	7440-09-7
Phosphoric acid and polyphosphoric acids	7664-38-2
Sulphur dioxide	7446-09-5
Aluminium hydroxide	21645-51-2
Commercial calcium hypochlorite and other calcium hypochlorites	7778-54-3
Hypochlorites (excl. of calcium) and chlorites; hypobromites	7681-52-9
Sulphides and polysulphides	1313-82-2
Sulphate of aluminium	7784-31-8
Sulphate of barium	7727-43-7
Sulphates other than of aluminium and barium	7778-18-9
Manganites, manganates and permanganates	7722-64-7
Silver nitrate	7761-88-8
Fulminates; cyanates and thiocyanates	628-86-4
Methanol (methyl alcohol)	67-56-1
Propan-1-ol (propyl alcohol) and propan-2-ol (isopropyl alcohol)	71-23-8
Butan-1-ol (n-butyl alcohol)	71-36-3
Other butanols, n.e.c.	78-83-1
Octanol (octyl alcohol) and isomers thereof	123-96-6
Allyl alcohol and other unsaturated monohydric alcohols (excl. acyclic terpene alcohols)	107-18-6
Ethylene glycol (ethanediol)	107-21-1
Cresols and their salts	1319-77-3
Industrial stearic acid	57-11-4
Industrial oleic acid	112-80-1
Palmitic acid	57-10-3
Stearic acid	57-11-4
Acetic anhydride	108-24-7
Lauric acid and others; salts and esters	143-07-7

PRODCOM entry	CAS number of substance evaluated
Lauric acid, salts and esters	143-07-7
Adipic acid, its salts and esters	124-04-9
Methylamine; di- or trimethylamine and their salts	124-40-3
Hexamethylenediamine and its salts	124-09-4
Monoethanolamine and its salts	141-43-5
Diethanolamine and its salts	111-42-2
Cyclohexanone and methylcyclohexanones	108-94-1
2,2-Oxydiethanol (diethylene glycol, digol)	111-46-6
Ammonia, anhydrous	7664-41-7
Ammonia, in aqueous solution	1336-21-6

Class E (n=41)

PRODCOM entry	CAS number of substance evaluated
Carbon dioxide	124-38-9
Copper oxides and hydroxides	1317-39-1
Sulphur; sublimed or precipitated; colloidal sulphur	7704-34-9
Boron; tellurium	13494-80-9
Sulphides of non-metals (excl. carbon); commercial phosphorus trisulphide	1314-85-8
Hydroxide and peroxide of magnesium, (hydr)oxides, peroxides of strontium or barium	1304-29-6
Chlorate of sodium	7775-09-9
Other chlorates,(per)chlorates, (per)bromates, (per)iodates	3811-04-9
Disodium carbonate	497-19-8
Potassium carbonates	584-08-7
Barium carbonate	513-77-9
Lithium carbonates	554-13-2
Sulphur (excl. crude; sublimed; precipitated and colloidal)	7704-34-9
Acyclic hydrocarbons, saturated	106-97-8
Ethylene	74-85-1
Cyclohexane	110-82-7
o-Xylene	95-47-6
p-Xylene	106-42-3
m-Xylene and mixed xylene isomers	108-38-3; 1330-20-7
Ethylbenzene	100-41-4
Cumene	98-82-8
Biphenyl, terphenyls, other cyclic hydrocarbons	92-52-4
1,2-Dichloropropane (propylene dichloride) and dichlorobutanes	78-87-5

PRODCOM entry	CAS number of substance evaluated
Saturated chlorinated derivatives of acyclic hydrocarbons, n.e.c.	540-54-5
Pentanol (amyl alcohol) and isomers thereof	30899-19-5; 123-51-3
Lauryl alcohol; cetyl alcohol; stearyl alcohol and other saturated monohydric alcohols (excl. methyl, propyl and isopropyl, n-butyl, other butanols, amyl, octyl)	112-53-8
Ethyl acetate	141-78-6
6-Hexanelactam (epsilon-caprolactam)	105-60-2
Butanal (butyraldehyde; normal isomer)	123-72-8
Vanillin (4-hydroxy-3-methoxybenzaldehyde)	121-33-5
Ethylvanillin (3-ethoxy-4-hydroxybenzaldehyde)	121-32-4
Aldehyde-ethers,aldehyde-phenols,aldehydes (other oxygen function) excl. vanillin (4-hydroxy-3-methoxybenzaldehyde), ethylvanillin (3-ethoxy-4-hydroxybenzaldehyde)	121-33-5
Acetone	67-64-1
Butanone (methyl ethyl ketone)	78-93-3
4-Methylpentan-2-one (methyl isobutyl ketone)	108-10-1
Diethyl ether	60-29-7
Ammonium chloride	12125-02-9
Ammonium carbonates	1111-78-0
Ammonium nitrate (excl. in tablets or similar forms or in packages of a weight of <= 10 kg)	6484-52-2
Sodium nitrate, natural	7631-99-4
Sodium nitrate, other	7631-99-4

9.5. Annex 5: Mapping of the new dataset ENV_CHMHAZ with the new codes and labels towards the old version

The chemicals are assigned to five aggregated classes according to their specific toxicity (for the indicator 'Production of toxic chemicals') and to their environmental classes (for the indicator 'Production of environmentally harmful chemicals').

The current Statistical working paper was ready to be published when the new dataset 'Production and consumption of chemicals by hazard class' (ENV_CHMHAZ) was published on the Eurostat Database. The naming of the classes has been revised in order to be consistent with other datasets of Eurostat. This harmonization has no impact on the methodological definition of the classes, i.e. only the names have been adjusted.

Table 15 shows the mapping between the old toxic / environmental classes and the new hazard classes: hazardous to health / hazardous to the environment.

Table 155: Mapping of the new dataset ENV_CHMHAZ with the new codes and labels towards the old version

New code	New Label	Old code	Old label
HAZARD	Hazard class	BREAK_SD	Breakdown for sustainable development
HAZ_NHAZ	Hazardous and non-hazardous - Total	TOTCHEM	Total production of chemicals
HLTH	Hazardous to health	TOTTOX	Total toxic chemicals
HLTH_CMR	Carcinogenic, mutagenic and reprotoxic (CMR) health hazard	CMR	CMR - chemicals
HLTH_CHRTOX	Chronic toxic health hazard	CHRONIC	Chronic toxic chemicals
HLTH_VTOX	Very toxic health hazard	VERY	Very toxic chemicals
HLTH_TOX	Toxic health hazard	TOXIC	Toxic chemicals
HLTH_HRM	Harmful health hazard	HARM	Harmful chemicals
ENV	Hazardous to the environment	TOTHARM	Environmentally harmful chemicals, total
ENV_SGNACU	Significant acute environmental hazard	ACUTE	Chemicals with significant acute environmental impacts
ENV_SEVCHR	Severe chronic environmental hazard	SEVERE	Chemicals with severe chronic environmental impacts
ENV_SGNCHR	Significant chronic environmental hazard	SIGNIF	Chemicals with significant chronic environmental impacts
ENV_MODCHR	Moderate chronic environmental hazard	MDRT	Chemicals with moderate chronic environmental impacts
ENV_CHR	Chronic environmental hazard	CHRNC	Chemicals with chronic environmental impacts

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Compilation of chemical indicators

DEVELOPMENT, REVISION AND ADDITIONAL ANALYSES

This methodology paper aims to give a comprehensive description of the way chemical indicators have been developed by Eurostat. It explains the compilation process of the indicators on:
- Production of toxic chemicals;
- Production of environmentally harmful chemicals.

This methodology paper focuses on the first of these indicators, 'Production of toxic chemicals' and explains the methodological adaptations and revisions of the indicators that became necessary due to:
- the enlargement of the EU, most recently from EU-27 to EU-28 with the accession of Croatia,
- changes in the PRODCOM list, and
- changes in the hazard classification of chemical substances, triggered by the introduction of Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures (CLP Regulation), which form the basis of an assignment to a toxicity class.

For more informations
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