Emission estimation and REACH – data sources and their use

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Goal, Scope and Background. Emission estimation is an essential prerequisite for exposure assessment and risk characterisation. REACH, the future European regulation for industrial chemicals, requires for certain substances exposure scenarios as a main element of the chemical safety assessment. According to the present discussion, for most producers and importers of substances and preparations (not been involved so far in the assessment of new substances) emission estimation as well as exposure assessment seem to be completely new tasks.
Materials and Methods: To facilitate the use of already-existing data for exposure assessment under REACH, an emission estimation tool accompanied with an instruction manual is considered to be a welcome supplement for both industry and authorities. A project called "Branch- and product-related emission estimation tool for manufacturers, importers, and downstream users within the REACH-system" aimed to develop such emission estimation tools – on the basis of a documentation of existing data on emission estimation. Therefore a survey on available emission data in central documents has been made. This article presents main findings of the phase of this project referring to the analysis of existing emission estimation data.
Results: The references found have been documented by using a specific kind of matrix. In addition, a guidance how to find the appropriate emission data has been developed. For two industrial branches, stand-alone emission estimation IT tools have been developed.
Discussion: There is an impressive documentation about branch-specific emission situations publicly available in emission scenario documents (ESD) from several sources. They can be used as valuable data sources for the development of quantitative exposure scenarios for REACH. At present, there is only limited awareness about these data in the supply chains.
Conclusions: Emission scenario documents have been developed as support for the risk assessment of existing and new chemicals done by authorities. In order to use them for the registration duties under REACH by manufacturers, importers and downstream users, they have to be adapted to the specific structure of the supply chains. In addition, they need to be "translated" into the branch-specific terminology.
Recommendations: The transfer of existing knowledge into the REACH system requires communication and exchange with the actors in these branches. This can be supported by authorities, but should be done mainly by the actors of the supply chains. A structured communication of safe conditions of use will become one of the central elements of a successful implementation of REACH.
Perspectives: The results from the work on plastic additives and photochemicals in the matrix project might be useful as a blueprint for similar tool developments in other supply chains. Calculation tools for emission estimation which have been elaborated together with the actors of the industrial branches can become an important element for a successful implementation of REACH.

Key words: emission estimation, emission scenario documents, emission estimation module, ESD matrix, OECD, REACH, sustainable chemistry, sustainable management of chemicals, supply chains, communication.

Emission estimation and REACH

Emission estimation is an essential prerequisite for exposure assessment and risk characterisation. REACH, the future European regulation for the registration, evaluation, authorisation and restriction of chemicals, requires for certain substances exposure scenarios as a main element of the chemical safety assessment. According to the present discussion, for most producers and importers of substances and preparations (not been involved so far in the assessment of new substances) emission estimation as well as exposure assessment seem to be completely new tasks (even if they could be known at least partly from the management of dangerous substances already today).

There is an impressive documentation about branch-specific emission situations publicly available in emission scenario documents (ESD) from several sources. They can be used as valuable data sources for the development of quantitative exposure scenarios for REACH.

At present, there is only limited awareness about these data in the supply chains. The EU TGD and the OECD ESDs are rarely known or used in the existing supply chains – in spite of the fact, that the OECD ESDs have been developed in cooperation with companies and industry associations. Therefore the use of this information by the actors of REACH requires intensive communication work.
Emission scenario documents have been developed as support for the risk assessment of existing and new chemicals done by authorities. In order to use them for the registration duties under REACH by manufacturers, importers and downstream users, they have to be adapted to the specific structure of the supply chains. In addition, they need to be "translated" into the branch-specific terminology. This requires communication and exchange with the actors in these branches.

The OECD Matrix project

In order to support the use of already-existing emission estimation data for the exposure assessment required under REACH, the OECD matrix project has been performed. It has the overall objective to develop technical guidance documents (manual and software tools) for emission and subsequent exposure estimation. Such guidance has to be robust and easy to use by manufacturers, importers and downstream users of substances. The conceptual approach has been based on the methodology laid down in EU TGD on Risk Assessment of New and Existing Substances (2003) and the OECD Emission Scenario Documents (ESD).
Within the project part B1, a survey on available emission data in central documents has been made. The references found have been documented by using a specific kind of matrix. In addition, a guidance how to find the appropriate emission data has been developed. For two industrial branches, stand-alone emission estimation IT tools have been developed. The results of the project have been worked out in intense exchange with RIVM (National Institute of Public Health and the Environment, Bilthoven, The Netherlands). RIVM has developed a guidance how to find the appropriate emission scenarios (see final report of the matrix project, Umweltbundesamt 2006).
This article presents the main findings of the survey on publicly available emission data. The additional results from the other parts of the project have been published in the project report (Umweltbundesamt 2006).

1 Publicly available data on emissions of chemicals

Branch-specific data on emissions of chemicals are documented in several publications. The following two chapters describe in brief information, which were developed to support the risk assessment of chemicals (existing chemicals and new chemicals) and scenarios from the US EPA. Further sources are mentioned in chapter 1.3.

1.1 The EU Technical Guidance Document (TGD) and the OECD Emission Scenario Documents (ESDs).

The EU Technical Guidance Document (TGD) on Environmental and Human Health risk assessment (TGD 2003) and the OECD emission scenario documents contain a large amount of branch-specific emission data.
The general principles for risk assessment as laid down in Directives 93/67, 1488/94 and 98/8 do not include technical details on how to actually carry out the different steps of the risk assessment. Therefore the TGD provide extensive supplementary details from the hazard identification up to the risk characterisation. This includes description of exposure estimation. The TGD is issued by the European Commission, Joint Research Centre (DG JRC), Institute for Health and Consumer Protection, European Chemical Bureau.
The TGD is the official reference document for preparing comprehensive and detailed risk assessment reports of chemicals following the current EU legislation. At present, this is done by the Member States Competent Authorities. Under REACH, chemical safety reports will have to be prepared by manufacturers and importers of substances. A description of the methodology used for this purpose is actually developed in the REACH implementation project (RIP) 3.2-2. The methodology is mainly based on the principles laid down in the TGD.
The A-tables of the EU TGD contain release factors for 16 industrial categories regarding the different life cycle stages (mainly production, formulation and industrial use, some information for professional and private use as well as service life, waste disposal and recovery. The B-tables of the EU TGD give default values for the size of a local source (fraction of the main source) and the number of release days per year. In total, the EU TGD contains 31 A-tables and 47 B-tables. The following table 1 lists the industrial categories and examples for chemical products used in the respective branches.

Table 1: Industrial categories with examples (TGD 2003).

	Industrial category	Examples
IC1	Agricultural industry	Plant protection products; fertilisers.
IC2	Chemical industry: basic chemicals	Solvents; pH-regulating agents (acids, alkalis).
IC3	Chemical industry: chemicals used in synthesis	Intermediates (including monomers); process regulators.

IC4	Electrical/electronic engineering industry	Electrolytes; semiconductors. Not: galvanics; electroplating agents.
IC5	Personal/domestic	Professional products used in public areas as non-agricultural pesticides, cleaning agents, products used in offices, e.g. correction fluids, printing inks.
IC6	Public domain	E.g. Professional products used in public areas as non-agricultural pesticides, cleaning agents, products used in offices e.g. correction fluids, printing inks.
IC7	Leather processing industry	Dyestuffs; tanning auxiliaries.
IC8	Metal extraction industry, refining and processing industry	Heat transferring agents.
IC9	Mineral oil and fuel industry	Gasoline; motor oil; gear oil; hydraulic fluid; colouring agents; fuel additives; antiknock agents; waste oil detoxification agents.
IC10	Photographic industry	Antifogging agents; sensitisers.
IC11	Polymers industry	Stabilisers; softeners; antistatic agents; dyestuffs.
IC12	Pulp, paper and board industry	Dyestuffs; toners.
IC13	Textile processing industry	Dyestuffs; flame retardants.
IC14	Paints, lacquers and varnishes industry	Solvents; viscosity adjusters; dyestuffs; pigments.
IC15	Engineering industry: civil and mechanical	Agents used in construction work, in automobile, aircraft and ship building.
IC16	Others	Substances not described elsewhere.

Supplementary to the EU TGD, the OECD Task Force on Environmental Exposure Assessment (TFEEA) develops Emission Scenario Documents ("ESDs") since 1998. An Emission Scenario Document is defined as a description of sources, production processes, pathways and use patterns with the aim of quantifying the emissions (or releases) of a chemical from production, formulation, use (industrial use, professional use, private use of chemical substances/preparations), service life (use in articles) and recovery/disposal into water, air, soil and/or solid waste. It has been discussed to prepare ESDs only for selected life cycle stages.
The OECD Emission Scenario Documents published so far contain a lot of branch-specific data on processes, chemicals used and emission patterns. These documents focus on emissions to the environment. Only in a few cases, emissions and exposures of humans (occupational health) are considered, too[1]. Information on ESDs used in national or regional context is compiled in the OECD Database on Use and Releases of Chemicals (http://www.oecd.org).

1.2 Generic scenarios and OPPT spreadsheets

The Office of Pollution Prevention and Toxics (OPPT) of the US EPA has prepared generic emission scenarios for several industrial branches. A compilation of generic scenarios can be downloaded from the Exposure Assessment Guidance website of the USEPA.[2]
The generic scenario compilation consists of pdf-documents containing written and graphic information about the industrial processes to be assessed. Besides the process technology, the occupational exposure and the environmental releases are described. In addition some scenarios give examples of how the exposure levels and release rates can be calculated. Some of the information given, however, like the data on market shares or the number of industrial sites, refers particularly to the conditions present in the US. On the basis of these generic scenarios the New Substances Branch of Environment Canada elaborated the so-called OPPT spreadsheets, the name coming from the USEPA office that issued the original scenarios. The Excel-file containing all OPPT spreadsheets is available on the website of the Task Force on Environmental Exposure Assessment of the OECD Risk Assessment Programme.[3]
Currently 32 of the existing 58 generic scenarios have been adapted to the spreadsheet format (see table 2). Some follow-ups are still required. The background information about the industrial process given in each spreadsheet is more reduced than the information given in the respective generic scenario. The information about occupational exposure is not included at all. Being part of an Excel-file the OPPT spreadsheets permit the automatic calculation of the release rate to the aquatic medium. If relevant, information about the air release calculation is also given. Based on the calculated release to water and on a set of flow rate data from Canadian rivers and lakes the PEC in these specific aquatic systems is determined.

Table 2: US EPA generic scenarios available as OPPT spreadsheet.

scenario #	scenario
A-1-6	Adhesives Manufacturing
AB-1-2	Leather Tanning
AC-1-4	Leather Dyeing
AD-1-19	Lube Oil Additives
AE-1-11	Metal Cleaning and Degreasing - Vapour Degreasing
AF-1-5	Metal Cleaning / Degreasing - Semi-aqueous Cleaners
AH-1-11	Paper Dyes - Manufacture and Use of

[1] E.g. OECD emission scenario document on photoresist use in semiconductor manufacturing (OECD 2004/9).
[2] http://www.epa.gov/opptintr/exposure/docs/guidance.htm
[3] http://webdomino1.oecd.org/comnet/env/RiskAssess.nsf

AI-1-9	Pesticides - Agricultural
AJ-1-9	Pesticides - Non-Agricultural
AO-1-3	Petroleum Refining - Crude Refining & Catalytic Cracking
AR-1-7	Printing Inks - Newspaper Printing
AS-1-9	Printing Inks - Manufacture & Use of Printing Inks
AT-1-13	Surfactants - Granular Detergents Manufacture
AU-1-3	Surfactants - Household Cleaners
AV-1-10	Surfactants - In Industrial/Commercial laundries
AW-1-12	Synthetic Fiber manufacture
AX-1-7	Textiles - Fabric Finishing
AY-1-16	Textiles - Textile Dyeing
AZ-1-2	Toner Used in Photocopier
BA-1-5	Water Cooling Towers Chemicals
BB-1-6	Water Treatment - Coagulants
BC-1-7	Water Treatment Disinfectants - Application
BD-1-6	Wood Preservatives - Appl. of waterborne using pressure treatment
BE-1-4	Wood Preservatives - Formulation of water soluble
C-1-5	Carbonless Copy Paper
E-1-9	Emulsion/Formulation of Latex
F-1-23	Automotive Spray Application
F-24-46	Control Technology-Auto Refinishing
G-1-2	Furniture Spray Application
Q-1-7	Coatings - Electrodeposition
R-1-16	Electroplating for Metal Treatment
Y-1-10	Fragrances - Manufacture and Use Of

Most of the generic scenarios and consequently of the OPPT spreadsheets describe processes belonging to the professional use life cycle stage of a substance or, to a lesser extent, to the life cycle stage of formulation.

1.3 Further documents containing emission estimation data.

There are further documents publicly available with relevance for emission estimation in several branches. Examples are CLEANTOOL: integrated assessment tool for cleaning processes in the metal industry (Kooperationsstelle Hamburg), ConsExpo (Advanced model for consumer exposure, developed by RIVM), COSHH Essentials (control guidance sheets, risk management, working place) and the standard exposure scenarios for isocyanates in TRGS (Technische Regel für Gefahrstoffe) 430. More examples are listed in Annex 8 of Supplement 2 of the Matrix report.

2 Structural analysis of central documents and the ESD matrix

In the matrix project, the A-and B-tables of the TGD and eleven OECD emission scenario documents have been analysed in detail. The objectives of this analysis have been:

- identification of common and branch-specific structural elements necessary to describe the emission of chemicals (see chapter 3 of this article);
- structuring of emission data from central documents in a form which supports their use by actors of the supply chains involved in REACH.

Table 3 lists the OECD emission scenario documents, which have been analysed in the matrix project.

Table 3: OECD emission scenario documents analysed in the matrix-project.

Plastic additives (OECD 2004/3)	Lubricants and lubricant additives (OECD 2004/10)
Photographic industry (OECD 2004/5)	Coating application via spray-painting in automotive refinishing (OECD 2004/11)
Rubber additives (OECD 2004/6)	Metal finishing (OECD 2004/12)
Textile finishing industry (OECD 2004/7)	Metal processing (Draft, Baumann et al. 1999)
Leather processing (OECD 2004/8)	Paints, lacquers and varnishes in coatings industry (draft, OECD 2003)
Photoresistant use in semiconductor manufacturing (OECD 2004/9)	

Additional to the documents analysed, there are some related documents, which have not been included in the matrix project (published OECD emission scenario documents as well as not yet OECD-published drafts). They

refer to industrial surfactants, pulp and paper industry, printing industry, chemical industry, blending of fragrance oils into consumer and commercial products, transport and storage of chemicals, Canadian scenarios on mills (wool, woven, carpet, knit).

Structuring the information of a single document. For each of the analysed documents, an Emission Scenario Profile (ES profile) has been prepared. These profiles give a first overview on the structure and the contents of the documents. Emission scenario documents often describe several emission situations ("scenarios"). In order to support the use of this information, such subsets of data, referring to a specific emission situation, have been identified in the analysed ESDs. These subsets are called "emission estimation modules" (EEMs).

For an individual emission scenario document, the emission estimation modules are documented in a structured manner using the so-called "mini-matrix". It shows directly which life cycle stages and which environmental compartments are addressed by emission estimation data. An example referring to the OECD emission scenario document on plastic additives (OECD 20004/3) is given in the following figure 1. This document describes in total ten different emission situations. They are labelled as emission estimation modules EEM 11.1 – EEM 11.10. These data sets refer to the estimation emissions to the environmental compartments water and air during four life cycle stages (raw materials handling and formulation, industrial use (processing/conversion), service life, waste/recovery). The life cycle stage "private use" has not been discussed within the ESD. (Because default values for the production step are given in the related A- and B-tables of the TGD, data for the estimation of emission related to the production of the plastic additives are not given in the ESD of the OECD).

	Production	**Raw materials handl. formulation**		**Industrial use / processing / conversion**	**Private use**	**Service life**	**Waste / recovery**
Water	Not discussed in the OECD emission scenario document (see TGD A- and B-tables)	EEM 11.1	EEM 11.3	EEM 11.5	Not discussed in the OECD emission scenario document	EEM 11.7	EEM 11.9
Air		EEM 11.2	EEM 11.4	EEM11.6		EEM11.8	EEM 11.10
Soil							
Waste							

Fig. 1: Mini matrix for the OECD Emission Scenario Document on Plastic additives (OECD 2004/3), IC 11 Polymers Industry.

A structured overview as given in Fig.1 facilitates the use of emission scenario documents. Therefore we recommend to introduce such a table in the emission scenario documents, which are developed in future.

Structuring the information of all analysed documents: The eleven OECD ESDs which have been analysed in detail contain in total 62 emission estimation modules. These modules describe emissions of chemicals to several environmental compartments during different life cycle stages.

In order to have an overview, which data sets are available for specific industrial categories (ICs) and life cycle stages, all emission scenario modules from the analysed Emission Scenario Documents are allocated within a matrix, the so-called "ESD Matrix".

This matrix shows for each industrial category, which A- and B-tables of the TGD are relevant and whether there are additional information available from OECD emission scenario documents. If this is the case, a short description of the module as well as the reference are provided in the report of the OECD Matrix project. A short version of the Matrix is given in Table 4.

The emission data available for plastic additives refer to industrial category (IC) 11. In the corresponding line of the ESD matrix the ten emission estimation modules of the OECD Emission Scenario document (see fig 1) are cited in the specific cells of the life cycle stages. In addition it can be seen that the TGD contains for the polymer industry in total three A-tables and eight B-tables. These tables can be used as sources for default values if no data are given in the OECD emission scenario document or if no site-specific data are known.

Table 4: The ESD Matrix – Allocation of A- and B-tables and emission estimation modules (EEMs).

IC		Production	Formulation	Industrial use	Private use	Service life	Recovery	Waste disposal
1	**Agricultural industry**							
	A-tables	A1.1	A3.1					
	B-tables	B1.1-B1.4	B3.1					
2	**Chem. industry: basic chemicals**							
	A-tables	A1.1	A3.2					
	B-tables	B1.1, B1.5	B3.2					
3	**Chem. industry: chemicals used in synthesis**							
	A-tables	A1.1-A1.2	A3.3					
	B-tables	B1.2, B1.6	B3.2					

IC		Production	Formulation	Industrial use	Private use	Service life	Recovery	Waste disposal
4	**Electrical / electronic engineering industry**							
	A-tables	A1.1	A2.1	A3.4				
	B-tables	B1.6-B1.7	B2.3-B2.4	B3.2				
	EE Modules			4.1-4.5				
5	**Personal/domestic**							
	A-tables	A1.1, A1#	A2.1, A2#		A4.1			
	B-tables	B1.6-B1.7	B2.1, B2.3		B4.1, B4#			
6	**Public domain**							
	A-tables	A1.1, A1#	A2.1, A2#	A3.5				
	B-tables	B1.6-B1.7	B2.1, B2.3	B3.3				
7	**Leather processing industry**							
	A-tables	A1.1, A1.3	A2.1	A3.6				
	B-tables	B1.4, B1.8-B1.9	B2.3-B2.4, B2.6	B3.4				
	EE Modules			7.1				
8	**Metal extraction industry, refining and processing industry**							
	A-tables	A1.1	A2.1-A2.2	A3.7				
	B-tables	B1.2, B1.4, B1.6, B1.10	B2.3-B2.4	B3.5-B3.6				
	EE Modules			EEM 8.1				
	EE Modules, Lubricants		8.2		8.3			
9	**Mineral oil and fuel industry**							
	A-tables	A1.1	A2.1	A3.8	A4.2			
	B-tables	B1.1-B1.2, B1.4, B1.11	B2.6-B2.8	B3.7	B4.1			
10	**Photographic industry**							
	A-tables	A1.1	A2.1, A2.3	A3.9	A4.3			A5.1
	B-tables	B1.4, B1.12	B2.3, B2.8	B3.8	B4.2			B5.1
	EE Modules			EEM 10.1-2			EEM 10.3	
11	**Polymers industry**							
	A-tables	A1.1	A2.1	A3.10-A3.11				
	B-tables	B1.4, B1.9, B1.13-B1.14	B2.3, B2.8-B2.9	B3.9				
	EE Modules, Plastic Additives		EEM 11.1-11.4	EEM 11.5-11.6		EEM 11.7-11.8		EEM 11.9-11.10
	EE Modules, Rubber Additives		11.R.1-11.R.2	11.R.1-11.R.2		11.R.3		
12	**Pulp, paper, and board industry**							
	A-tables	A1.1, A1.3	A2.1	A3.12-A3.13				A5.2
	B-tables	B1.4, B1.8-B1.9	B2.1, B2.3, B2.8	B3.10				B5.2
13	**Textile processing industry**							
	A-tables	A1.1, A1.3	A2.1	A3.14	A4.4			
	B-tables	B1.2, B1.6	B2.3, B2.10	B3.11-B3.12	B4.3			
	EE Modules			EEM 13.1-4		EEM 13.5		
14	**Paints, lacquers, and varnishes industry**							
	A-tables	A1.1	A2.1	A3.15	A4.5			
	B-tables	B1.2, B1.6	B2.3, B2.10	B3.13	B4.4-B4.5			
	EE Modules		14.1-14.9	14.10-14.23	14.12	14.10-23		14.1-24
	EE Modules, Automotive coating			14.A1-14.A6				
16	**Engineering industry: Civil and mechanical**							
	A-tables	A1.1	A2.1	A3.16	A3.16			
	B-tables	B1.2, B1.6	B2.3, B2.8	B3.14	B4.5			
	EE Modules, Automotive coating: see under IC 14.							
0/15	**Others**							
	A-tables	A1.1	A2.1	A3.16				
	B-tables	B1.2, B1.6	B2.3, B2.8	B3.14	B4.5			B5.3

The extended version of the ESD Matrix contains references for all data sets mentioned in the matrix. The extended version is part of the OECD Matrix project report.
At present, the ESD matrix refers to data sets of the TGD and the OECD ESDs analysed in the matrix project. Emission estimation data from other sources (e.g. from the OPPT spreadsheets) can also be documented as emission estimation modules and be allocated to specific cells of the ESD Matrix.

3 Characteristics of the OECD emission scenario documents

Differences and similarities. The analysed OECD ESDs show a broad variety regarding

- Number and complexity of industrial branches covered;
- Number and complexity of processes covered;
- Life cycle stages covered;
- Detailed description of types of chemicals used and their emission behaviour;
- Detailed description of typical point sources, including size and emission patterns;
- Description of branch-specific and process-specific emission drivers.
- Number of emission scenarios;
- Structure of the emission rate formulas.

A short structural characterisation of the OECD ESDs regarding the aspects mentioned above is given in the related ES profiles (see final report of the matrix project). A deeper structural analysis has been made with some of the OECD ESD, looking especially for the relevant emission drivers and related default values.
The OECD ESD (draft) on paints, lacquers and varnishes (OECD 2003) is a good example for a document covering a broad range of industrial applications, from internal lacquering of beverage cans (EEM 14.17 and EEM 14.18) up to the application of coil coatings (EEM 14.20) and the application of marine coatings (EEM 14.21). Just the opposite, the OECD draft on automotive refinishing (OECD 2004/11) describes exclusively one specific process (spray-painting) (EEM 14a.1-EEM 14A.6). The other emission scenario documents are located in between these two examples. The document on lacquers and varnishes gives highly aggregated emission estimations (OECD 2003). In such cases it is difficult to identify the single emission drivers contributing to the total emission. Branch-specific data are given in all so far analysed ESDs.

Emission estimation formula: The amount of a chemical, which is emitted from a production process, depends in general on the following factors:

- The physico-chemical properties of the substance;
- The amount of the chemical used in the process (if it is part of a chemical product, the amount is depending on its concentration and the amount of the chemical product used);
- The percentage of the amount used which is not consumed or converted during the process, but emitted;
- The application of abatement techniques used in order to reduce the emission of chemicals.

As a generic starting point for the emission estimation a general formula can be used which takes these factors into account:

$$E = \frac{Q_{product} \cdot C_{chemical} \cdot F_x \cdot \prod_{j=1}^{n} \left(1 - F_{abatement,j}\right)}{T_{emission}}$$

E	emission rate [kg.d^{-1}]
$Q_{product}$	the quantity processes or used per time period [kg.yr^{-1}] (data from ESD)
$C_{chemical}$	the concentration of the chemical in the product [kg.kg^{-1}] (data from ESD)
F_x	relevant emission factor [-] (from matrix emission module)
$F_{abatement}$	efficacy factor for abatement technique (RMM) [-] (from ESD, model or database)
$T_{emission}$	the emission period [d.yr-1] (from ESD or B-table of EU TGD)

In some cases, the emission rate formulas contain branch-specific factors. E.g. are the raw hide-reduction factor for leather industry (“fraction of remaining mass from raw hide”, EEM 7.1, OECD 2004/8), the fraction of photoresist adhering to the wafer in semiconductor manufacturing (EEM 4.1-4.5, OECD 2004/9) and the spray

gun transfer efficiency (OECD 2004/11). In these cases, the emission estimation can be adapted to the branch-specific situation by including these elements in the generic formula.

Scale: The emission estimation modules of the OECD Emission Scenario Documents address local as well as regional emissions. For the life cycle stages production, formulation and industrial use, a local concentration is estimated, based on the production volume of the registrant. Additionally, a regional background concentration can calculate based on 100% of the European production volume. For substances in wide disperse use (private use) or for emissions from service life of articles safety is assessed for the regional scenario.

Interface to appropriate fate models: The OECD ESDs concentrates on emission estimation. Interfaces to environmental fate models are described in some cases for the aquatic environment. Calculations of the PNEC are included in the OECD document on photochemicals. Fate models are described in detail, e.g. in the EU TGD (2003).

Covering of life cycle stages: Most of the emission estimation data identified from OECD ESDs refer to the life cycle stages formulation and industrial use. In all cases, for estimations during the production of the chemicals, the appropriate A- and B-tables of the TGD have to be considered. For all other life cycle stages, A- and B-tables as well as emission estimation data from OECD ESDs are available only in some cases (see the ESD matrix, annex 1. For an overview on available A- and B-tables, see annex 2 and annex 3).

The life cycle stage "professional use" is not addressed explicitly in the A- and B-tables of the TGD, neither in the OECD ESDs. For the life cycle stage "Private use", five A-and six B-tables are available. For the application of decorative paints (IC 14), an additional emission estimation module for general public use is available (EEM 14.12).

For the life cycle stages "service life" and "recovery", no A- and B-tables are available. The OECD ESDs on plastic additives (OECD 2004/3), on rubber additives (OECD 2004/6) and on textile finishing (OECD 2004/7) describe different types of emissions during service life. Emissions during recovery of chemicals are described for photochemicals (EEM 10.3, OECD 2004/5).

Branch- or company-specific abatement measures: Internal and external risk management measures are one of the key factors determining emissions. The measures can be branch- or process-specific. Under REACH, abatement techniques are part of the risk management measures. Abatement measures can include industrial or municipal waste disposal and waste water treatment. It can be distinguished between general applicable abatement measures vs. substance or process specific measures (e.g. removing heavy metals from electroplating solutions). The measures can be integrated, end-of-pipe, on-site or external. In each life cycle stage, abatement techniques can be relevant.

The OECD ESDs do not consider abatement measures in a uniform matter. In some documents, general or branch specific abatement measures are listed (e.g. clean room conditions, use of closed systems (OECD 2004/9, OECD 2004/11), good house keeping (OECD 2004/10), dust filters, VOC treatment, vacuum cleaners, (OECD 2003). Only in single cases quantitative default values for the efficacy are given – for an example see the following table 5 with data from the OECD ESD on the coating industry (OECD 2003).

Table 5: Assumed values for the efficiency of the different emission treatment techniques during the manufacture of organic solvent borne coatings (batch size of 10.000 litres or greater, OECD 2003, p. 47).

Treatment	Efficiency of the capture device	Scrubbing efficiency
Dust filter	0.97	0.99
VOC treatment	0	0
Vacuum cleaners	0.90	1

More often, abatement measures are not described in detail – but during determination of release factors it is assumed that standard abatement techniques are applied. In the emission scenario for HPV intermediates (EU TGD, 2003), in-plant-treatment (e.g. activated carbon treatment and precipitation) is already included in the factors. In these cases it is not possible to identify specific abatement-factors for the modelling of the emission situation. In some cases it is not clear, whether wastewater treatment is included in the emission estimations or not.

This difficulty regards end-of-pipe-measures and - to an even larger extend - process-internal and integrated measures. Integrated pollution prevention measurers are more difficult to quantify compared to onsite-pollution control. Integrated pollution and prevention control (IPPC) standards aim at minimising the primary losses from processes (prevention) and optimising the overall efficiency of secondary abatement techniques. This usually includes choices to which extent abatement takes place at production sites, at public wastewater treatment plants or at special waste treatment facilities (including recycling). Where and at which rate the emission takes place at

the end, is a question of environmental legislation and costs. This kind of "industrial waste processing" is not yet well reflected in the TGD supply chain model, neither the subsequent methodology in the OECD ESDs.

Abatement factors: For the emission and the exposure assessment under REACH, risk management measures are an important interface for responsibility. Within an exposure scenario, the manufacturer describes how he controls exposure and which measures he recommends downstream users to take. As a consequence, consideration of abatement measures becomes an essential element of emission estimation. Regarding the present situation of abatement factors within ESDs, the following recommendations are made:

- It should be clearly indicated whether published ESDs contain quantified abatement-factors.
- For standard techniques of risk management, standard values for efficacy should be determined in order to be used as default values within emission estimates. It is recommended to use standard measures as reference points, not maximum measures. If possible, values for best available techniques can be given additionally (for refinement options).
- Packages of abatement measures (and corresponding factors for packages) are more appropriate than a huge number of specific, stand alone measures. Packages/ cluster modules (combinations of individual measures) give more degrees of freedom to select individual measures without the need to communicate them. Abatement techniques are part of the risk management measures.
- It would be a great advantage to get the knowledge from down-stream companies on their standard measures currently applied into the system (inventory of possible techniques/techniques-in-use). The emission estimation tools should support the use of this knowledge for the emission estimation work.
- It would be helpful to have stand alone ESDs for external abatement techniques rather than addressing external abatement in UC-ESDs or IC-ESDs.

Possibilities to include the effect of risk management measures into the emission estimations have been elaborated exemplarily in the two supply chains chosen for IT tool development in the OECD Matrix project (see project report and the developed tools (www.emissiontool.com)).

6 Recommendations: the further development of emission scenario documents and their use

For quite a number of industrial uses of substances, emissions to the environment can be estimated based on the available OECD documents and the TGD, although the information is not presented yet in a user friendly way and the structure does not fit yet to the Exposure Scenario approach under REACH. The matrix project was initialised to make this information better accessible.

Based on the results of the phase B1 of the matrix project, we developed a number of recommendations. They refer to the further development of emission scenario documents in order to support the use of these data for emission estimations under REACH.

The distinct emission scenarios of an emission scenario document (ESD) could be marked as emission estimation modules. A mini-matrix (see fig. 1) can show at a glance which life cycle stages and which environmental compartments are addressed and can be included in an ESD. In addition, each ESD should include a table to show which industrial categories, use categories, risk management measures and process types have been taken into consideration.

There is a clear need to fill gaps and to update or refine the emission estimation modules currently available. Data on the emission pattern in space and time (duration, frequency, special distribution, emissions during service life) should be part of ESDs in future. Risk management measures should be addressed clearly in emission estimates. A list of standard techniques including default values for efficacy would be a very useful instrument. However, some risk management measures are integral parts of process design and process management. Such cases, where the emission factor already reflects parts of the risk management should be clearly flagged in the ESDs.

The industrial category "Others" (IC 0/15) should be diversified (approximately 40% of the industrial applications belong to this category).

New identified emission estimation modules can be allocated to the ESD matrix. This matrix can serve as a reference point for the selection of appropriate data sets for emission estimation.

The REACH-related work on emission estimation tools should be closely connected to the international work of the OECD Task Force on Environmental Exposure Assessment /TFEEA). Beside the OECD Emission Scenario Documents, also other comparable documents could be used to develop the tool-boxes for implementation of REACH, for example the OPPT generic scenarios (see chapter 1.2).

The existing data on emissions of chemicals (ESDs and their emission estimation modules) should be transformed into an electronic library system. From this system, the substance manufacturer can learn about the conditions of use and the factors driving the emission in his markets. Measures suitable to ensure safe use can be selected from this system. These library systems need a navigation system, to identify the most appropriate

module for a certain combination of preparation type, industry sector, life cycle stage, substance function and substance properties and process type.

In order to support the calculation of the emissions depending on the process type, the conditions of use and the measures applied, stand-alone IT tools should be developed. This has been done as part B2 of the matrix project for two supply chains: for plastic additives and photochemicals. (see www.emissiontool.com). The results from the work on these two examples might be useful as a blueprint for similar tool developments in other supply chains.
(Contact to receive the complete final report of the matrix project: silke.mueller@uba.de, d.bunke@oeko.de, reihlen@oekopol.de).

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