UBA R+D Project FKZ 204 67 456

(financed by Umweltforschungsplan of the German Federal Environment Ministry)

RIVM Project No. M/601200007

(financed by The Netherlands Directorate General of Environmental Protection)

Branch- and product-related emission estimation tool for manufacturers, importers, and downstream users within the REACH-system

OECD Matrix Project

Part A: Technical Guidance for identifying an appropriate emission scenario
Part B: Technical Guidance for emission estimation: manual and software tool

Summary Report

March 2006

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Project part A: Technical Guidance for identifying an appropriate emission scenario

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This publication is part of the OECD Matrix Project (“Branch- and product-related emission estimation tool for manufacturers, importers, and downstream users within the REACH-system”, UBA R+D Project FKZ 204 67 456 and RIVM Project No. M/601200).

The **summary report** contains the main results of the OECD Matrix Project.

The following reports are available and refer in detail to specific parts of the OECD Matrix Project:

- Developing the Target Funnel [project part A; RIVM Report No. 601200006, UBA-Text No. 10/06]
- Developing the ESD Matrix [project part B1]
- The ESD matrix [project part B1]
- Manual: Emission estimation for plastic additives [project part B2]
- IT system Manual (Part I); IT design document (Part II) [project part B2]
- Documentation: Emission estimation for photo-chemicals [project part B2]

The detailed reports are available as a zip-file. Please contact us.

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List of Abbreviations

CSA	Chemical Safety Assessment
EEM	Emission Estimation Module
EET	Emission Estimation Tool
ESD	Emission Scenario Document
ES	Exposure Scenario
IC	Industrial Category
MC	Main Category
PEC	Predicted Environmental Concentration
PNEC	Predicted No Effect Concentration
RMM	Risk Management Measures
TGD	Technical Guidance Document
UC	Use Category

1 Introduction

Over the last 10 years, the OECD Task Force on Environmental Exposure Assessment developed and published a number of Emission Scenario Documents (ESDs) on various industrial sectors. Some of the documents are included in the EU Technical Guidance Document on Risk Assessment (EU TGD, 2003; see chapter 7). As it was recognised that the ESDs are not well known outside of the authorities in the OECD Task Force the idea for a better communication of these document to the public arose. For the European member countries in the OECD this idea was also clearly connected to the technical implementation process of the new EU chemicals policy REACH.

The German Umweltbundesamt (UBA) took the initiative to launch the so-called ***Matrix*** project financed by the national research program of the Federal Environment Ministry (UFOPLAN FKZ 204 67 456). The project was conducted in close co-operation with the Dutch RIVM and co-financed by the The Netherlands Directorate General of Environmental Protection (Project No. M/601200). The project with the full title "Branch- and product-related emission estimation tool for manufacturers, importers, and downstream users within the REACH-system" started in July 2004 and finished in February 2006. A steering group with members from the OECD Task Force on Environmental Exposure Assessment, from industry and from further authorities was established for guiding the project.

The project is divided into two subprojects:

Project part A "Technical Guidance for identifying an appropriate emission scenario" was performed by the *Expertise Centre for Substances* of the Dutch RIVM, Bilthoven. Project part B "Technical Guidance for emission estimation: manual and software tool" was conducted by a German consortium of *Oeko-Institut e.V.,* Freiburg*, Ökopol GmbH,* Hamburg, and *ChemieDaten*, Strachau.

The outcome of the project in brief:

- Overview on the industry sectors and chemical product types for which Emission Scenario Documents exist: It is specified which life cycle stages and environmental compartments they cover. For the time being, the overview is presented as a matrix with single emission estimation modules (ESD matrix) including an explanatory guidance on how to make practical use of it. At the conceptual level, the matrix may serve as a starting point to develop an IT based library system for available emission estimation modules (EEM)[1]. Such modules may be loaded into an Exposure Scenario builder and/or into a tool to carry out the CSA.
- A decision tree which guides the registrant under REACH in identifying the correct emission estimation modules when carrying out the safety assessment for substance manufacture, formulation, and the identified uses. This decision tree is called ***target***

[1] It is one of the core ideas of the project that emission estimation documents can be unitised into emission estimation modules (EEM). In the current project, the EEM is defined as a base unit of the Emission Estimation Tool (EET), addressing a specific emission situation at a certain life cycle stage.

funnel and is presented as a potential element in the relevant industry workflows developed in RIP[2] 3.2 and RIP 3.5.

- IT tool for emission estimation for substances used in plastic additives, as an example how user-friendly tools for the emission estimation in a CSA could look like.
- Conclusions from testing the feasibility of transforming the emission estimation tool (EET) developed for plastic additives into an IT tool for another chain (photographic chemicals).
- A set of conclusions and recommendations related to further development of the ESD/EEM-matrix, the IT-tools, and the REACH implementation projects.

The final project reports can be downloaded under:

http://www.umweltbundesamt.de/uba-info-medien/index.htm

http://www.rivm.nl/bibliotheek/rapporten/

http://www.reach-info.de

http://www.emissiontool.com

2 Background

Under REACH, producers or importers of dangerous substances[3] with a market volume of more than 10 t per year are obliged to carry out a chemical safety assessment (CSA), including an exposure assessment. The result of the CSA is the Exposure Scenario (ES) which has to be communicated down the supply chain. The exposure scenario defines the operational conditions (including risk management) under which the use can be regarded safe. The exposure estimation is needed to demonstrate that the operational conditions of use and the risk management measures are suitable to limit exposure to a level well below the PNEC[4].

2.1 Exposure scenario and emission estimation under REACH

Under REACH, the Exposure Scenario describes the conditions under which a substance (as such, in a preparation or in an article) or a group of substances can be safely used. In this respect it has two functions:

- It is an element in the Chemical Safety Assessment based on which the exposure assessment and the risk characterisation is carried out.
- It is a mean for communicating operational conditions of use and risk management measures that are suitable to ensure adequate control of risk in the supply chain (ES integrated into the Safety Data Sheet (SDS) system).

[2] RIP: REACH implementation project
[3] Dangerous to human health or the environment, PBT or vPvB substance
[4] PNEC: predicted no-effect concentration

Both, the operational conditions of use (e.g. amount used, application process, duration and frequency of use) and the risk management measures (e.g. waste water treatment), together with the inherent properties of the substance (e.g. volatility, water solubility) determine the level of emission to a certain compartment. The volume of the receiving compartment (river water flow, indoor air exchange), again together with the substance' properties determines the level of exposure.

Once a registrant, has identified the relevant uses of his substance in the market and the broad conditions of use, he can derive a tentative exposure scenario and based on this assess the exposure and risk. Depending on the result one or more iterations of exposure estimation and risk characterisation may be carried out before the final ES can be defined. The whole process of ES development takes place in 8 steps (Figure 1). The emission estimation, exposure assessment and risk characterisation is needed to decide whether the conditions described in the ES ensure safe handling.

Steps in Developing an Exposure Scenario

1. Identify the use(s) for which an ES shall be developed
2. Describe manufacture or use in standard structure:
   - Life cycle stage
   - Type of technical process (e.g. dipping, spraying, coating, …) or article type (e.g. textiles, construction material)
   - Broad function of substance
   - Relevant routs of exposure
3. List the operational conditions (driving emission and exposure) as usually occurring in the market
4. List risk management measures typically applied in the market ..
   - …. under control of the manufacturer user
   - …. under external control (e.g. waste or waste water treatment)
5. Develop a tentative Exposure Scenario (referring to current practise)
   - Select a suitable name for the use/process addressed in the ES
   - Prepare a short process description
   - List the relevant operational conditions for which the ES is applicable
   - List which RMMs should be in place and which efficacy is assumed
   - List the determinants required for exposure estimates
6. Assess exposure and risk, decide on iteration strategy (if needed):
   - Carry out exposure estimate and compare with the PNEC
   - Decide how to proceed based on risk characterization
     - Collect more information on use and exposure or
     - tighten RMM or define a more narrow corridor for the operational conditions of use or
     - refine the hazard assessment; carry out additional testing; no further support of use;
7. Iterate the assumptions and derive the final Exposure Scenario following one of the options under 6.
8. Integrate the Exposure Scenario into the Safety Data Sheet

Figure 1: Steps for ES development[5]

[5] List compiled based on Report on RIP 3.2-1, 2005

2.2 The *Matrix* approach

The current project deals with the first essential step of the environmental exposure estimation only, the environmental emission estimation. This is since the tools for modelling the environmental fate of substances after release are available and work well.

The exposure assessment shall include all life cycle stages of a substance, the manufacture and own use of a substance as well as all further uses down the supply chain. Since the knowledge of the manufacturer on specific conditions of uses further down in the chain will usually be limited, the assessment method needs to be sufficiently robust to allow for generic assumptions and standardisation. Therefore, emission estimation should be built on four elements:

(a) a generic definition of factors driving the emission across all processes, products, sectors, or chains (common formula);

(b) a supply chain specific (and possibly life cycle stage specific) "expression" of these drivers determined by types of identified use, operational conditions of use, and risk management measures;

(c) an algorithm to translate operational conditions of use and risk management measures into quantitative estimates of emissions for a subsequent derivation of PECs[6];

(d) tools to enable and to encourage the actors in the supply chain to contribute relevant information in a "common language".

Sector specific reference documents on emission estimation exist at EU and OECD level (so-called emission scenario documents, ESDs), however, these have not yet been much used by industry since environmental safety assessment was not obligatory so far for most of the substances in the market. In order to provide guidance to industry how to make use of the existing information and tools under REACH, the OECD ***Matrix*** Project was launched.

3 A generic supply chain model for REACH

The IC/UC system of the current TGD has been analysed with regard to its suitability to structure emission estimation along supply chains (in products or processes).

The IC system of the TGD refers mainly to industry sectors, but it is not entirely consistent.

- Usually an industry category covers more than one life cycle stage, hence companies operating in the same industry category may belong to different industrial sectors (branches) or different supply chains respectively. The plastic conversion industry for example has close links to the final industrial users of plastic articles (e.g. car industry, building and construction, food industry). This is partly true also for the com-

[6] PEC: predicted environmental concentration

pounders. On the other hand, the manufacturers of additives, and again part of the compounders are typically organised in the Chemical Industry.

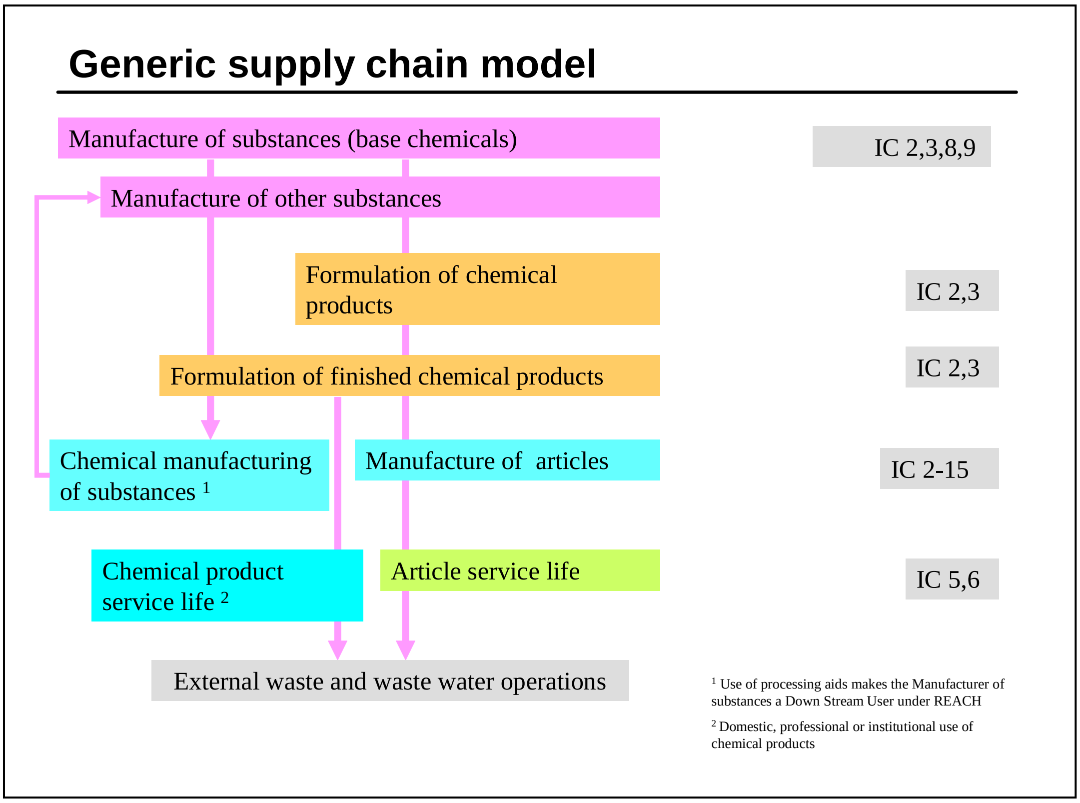
- The current definition of the industry categories (IC) is not entirely consistent in itself. Partly the name refers to the manufacture of chemical products (IC 14 paints, lacquers and varnishes industry), partly it refers to industrial manufacture of articles (IC 13 textile processing industry) and sometimes it refers to the manufacture of substances (IC 2, 3 Chemicals industry: basic chemicals and chemicals used in synthesis).

Also, the use category system of the TGD (UCs which describe technical function of a substance in a product or process) does not sufficiently fit into the REACH system yet. The technical function of the substance may be relevant for documentation under article 9 of REACH (registration dossier). However this may not necessarily be the case for communicating identified uses up and down the supply chain. Often substances are part of a "substance-package", and its technical function in the package may be seen as a business secrete by the manufacturer of this package (formulator).

The matrix design and the target funnel are based on a generic model of the supply chain (see figure 2). The current industry categories (ICs), the process categories (MC) and the life cycle stages of the EU Technical Guidance Document on Risk Assessment (TGD, 2003) have been assigned to this model and can be used to form 7 rather broad groups of emission estimation modules:

- Emissions from synthesising substances or extracting substances from crude oils, ores and other raw material taken from nature;
- Emissions from mixing substances with each other to manufacture chemical products (preparations) for a certain technical field of application;
- Emissions from using these chemical products in a wide range of industrial processes for manufacture of articles. The substance either becomes part of the article or is released with the waste water, air or (solid) waste;
- Emissions from using substances or preparation as processing aids in the synthesis of substances, refinery processes, or production of metals from ores;
- Emissions from using chemical products in private households and/or the public domain and/or small businesses (professional applications);
- Emissions from service life of articles into or onto which substances have been manufactured;
- Emissions from waste operations after service life.

Figure 2: Generic Supply Chain Model



4 The ESD matrix as a starting point for a library system

Within the EU TGD and the OECD emission scenario documents (ESDs), a large amount of branch-specific emission data has been published. They contain a lot of branch-specific data on processes, chemicals used and emission patterns mainly referring to releases to the environment.

Emission scenario documents often describe several emission situations (“scenarios”). In order to make this information better accessible, subsets of data referring to a specific emission situation have been identified in each of the analysed documents. These subsets are called “**emission estimation modules**” (EEMs).

In addition to the ESDs, the A- and B-tables of the EU TGD provide a generic emission estimation method based on the ICs and UCs and can be used as a safety net (if no more specific information is available).

In order to obtain an overview, which data sets are available for specific industrial categories (ICs) in relation to the substance’s life cycle stages, the emission estimation modules, together with the A- and B-tables, were allocated within the ESD matrix (see Annex 1). Each of the matrix cells represents a life cycle stage in a certain industry category. The EEMs in the matrix cells indicate for which process or product and for which environmental media generic release estimates are available. However, it does not yet allow to discriminate why an EEM is not available, whether it is a non-relevant exposure route, whether it is already covered by another EEM or whether an EEM has not yet been developed.

The matrix shows for each industrial category and life cycle stage, if and which A- and B-tables of the EU TGD are available and whether there are EEMs available from ESDs or from other sources in addition. If the latter is the case, a short description of the module as well as the reference are provided. The matrix is presented in Annex 1 of this report.

Based on this, the registrant could identify the information source containing suitable emission estimation modules and corresponding release factors for the life cycle of his substance.

The information sources identified through the cells (e.g. emission scenario documents) often contain more than one release factor per environmental compartment. Depending on the variety of processes and/or products covered, one cell of the matrix could also contain various EEMs. In principle it would be possible to systematically identify these sub-modules and the corresponding release factors when setting up a computerised library of EEMs. In such a system a single module may be characterised (labelled) with up to 7 identifiers:

- Industry category of final use of substance as such, in a preparation or an article [= IC of current TGD with some additional differentiation and restructuring where needed]
- Life cycle stage[7] [according to current TGD]
- Technical function of substance in a process or product [= current UC]
- Type of process [partly expressed as main category (MC) and partly expressed in the A-/B-tables of the current TGD]
- Size of source [= categories of processing capacity in the current A-/B-tables of the TGD]
- Type of chemical product and/or article in which the substance is contained when placed on the market for final use [the international trade codes for products could possibly be the basis for a category system]
- In addition, the EEMs may be indexed in accordance to which environmental medium it refers.

Product and process types are not yet consistently categorised in the current TGD. Such categories, however, may play a key role when communicating uses and conditions of use up and down the supply chain. Hence further development is needed here.

The system of identifiers can be structured in a hierarchical way among the identifiers and/or within one single identifier. Thus it will be possible to group a number of uses under broad categories by using generic identifiers or by applying only a subset of identifiers. (Standard) EEMs related to these broad categories will be based on conservative emission estimation. Such EEMs may be in particular suitable for carrying out a CSA at first or second iteration level derived for *Use and Exposure Categories* as defined in Article 3 (34) of the REACH proposal (politically agreed by the Competitiveness Council on

[7] Note that the professional use of a substance in small business is (from the environmental perspective) regarded as wide disperse use and hence treated in the same way like use in public domain and private households. However, from the occupational health perspective, “professional use” may be a category of its own.

December 13, 2005). Also, such a system of identifiers may be the basis to determine a standardised short title for a use or for an exposure scenario.

In practise, the number of different standard emission estimation modules for the life cycle stages “synthesis” and “formulation” may be relatively small as the processes involved are more or less similar between different industrial categories.

Also, for the service life of substances in articles a limited number of standard EEMs may be sufficient as a starting point, e.g.:

- Articles from which substances are released intentionally;
- Indoor use of articles (including discharge to municipal waste water and possibly exposure via indoor air);
- Outdoor use (including losses into the environment);
- Outdoor use under highly abrasive conditions (loss applications).

The highest diversity in conditions of use is to manage at the life cycle stage “industrial use”: This is illustrated in Table 1 by a combination of ICs (in the meaning of a group of typical manufacturing processes) and preparation types. In each of the cells a variety of application techniques will be relevant. These have partly a generic character and partly sector specific modifications. For example, paints, inks and coatings can be applied by a number of generic techniques. These usually differ from each with regard to the determinants of emissions, although belonging to the same product type and the same industry category: Spraying, rolling/brushing, printing, calandering, dipping/bathing. Vice versa, the emission drivers related to a certain application process may be quite similar even though different chemicals products and industry categories are involved.

Table 1: Uses identified by preparation type and sector specific manufacturing processes

	Private Household	Metal Finishing	Reprographic Industry	Polymer Industry	Textile Industry	Printing Industry	Vehicle Manufacture[8]
Dyes and inks	X			X	X	X	
Paints, coatings		X		X			X
Printing paste, textile coating				X	X	X	
Cleaners, washing agents	X	X			X	X	
Lubricants	X	X			X		X
Photochemicals	X		X				
Plating and galvanic agents		X					
Plastic additives and pigments				X			
Adhesives	X						X
Textile finishing products	X				X		

8 Other than covered already in metal finishing and polymer industry; not used as a stand alone IC in the TGD.

Processes with similar determinants and pathways of emission to the environment may possibly be reflected in one standard EEM, e.g.

- Manufacture of substances into or onto a matrix or removal of substances from a matrix in water (bath or flow) based processes (paper making, textile, leather, galvanisation):
- Conversion of polymers or metals (under elevated temperature);
- Manufacture of substances into or onto a matrix by spray application and subsequent drying;

Such clustering, however, is only possible, once the relevant emission processes have been described in a standard terminology and structure (see ESD matrix).

5 Workflow to identify suitable emission estimation modules

In order to derive exposure estimates and subsequent risk characterisation, the exposure determinants as identified in the Exposure Scenario (see step 5 in ES generation, Figure 1) must be linked with quantification mechanisms (as for example available in an IT based EEM-matrix or library). Information on these exposure determinants (e.g. the substance volume applied, the specific release factor in a process etc.) may be gathered from different sources: e.g. direct communication with the customers or with the downstream user organisations; retrieval of information from written information documents. The registrant's workflow will depend on the availability of structured information on the condition of use in the market segment where substance is applied. In cases, where no specific and REACH targeted information is available from downstream user organisations or his direct customers he may need to work with the information existing in EU or OECD Emission Scenario Documents or in the A- and B-tables of the EU TGD as a starting point.

However, because of the huge diversity in applications and functions, the selection of the appropriate emission scenario containing the relevant exposure determinants can be difficult, making the emission estimation one of the problematic areas in quantitative risk assessment of substances. Therefore, a tool has been developed for manufacturers, importers and downstream users of chemical substances to facilitate the selection of the appropriate emission scenarios with the best estimates for emission factors and emission period(s). This tool is called ***Target Funnel***.

The tool supports the selection of emission estimates to wastewater, air and soil for all relevant functions and life cycle stages, e.g. production, formulation, industrial use etc., in all possible applications and processes throughout industry and society.

The crucial part of the tool is the interactive generic decision tree leading to the required location (cell) in the ESD matrix of emission estimation modules (EEMs).

The routing through the decision tree is determined by selecting the right identifiers for each life cycle stage. The identifiers used agree with the identifiers defined for the EEMs (see chapter 4). Based on expertise and a thorough study of processes in the various life cycles of substances, at least 10 potentially relevant identifiers in the decision tree, such as the relevant industrial category, use category, the type of chemical product and semi-finished preparation (additive package), were determined to cover a complete life cycle of a substance. Where possible, these identifiers were supported by comprehensive pick lists.

The methodology has been tested and illustrated for two substances in different industrial categories. The first one concerns a (fictitious) anti-halo agent used in the preparation of photographic colour films and corresponds to a photochemical (Use Category (UC) 42) in the photographic industry (Industrial Category (IC) 11). The second one is a (fictitious) colouring agent in plastics used in pigment pastes (preparation) and master batches (chemical product) in the polymers industry (IC 11). The general structure of the target funnel and the application are presented in annex 2.

For both tests the routing through the decision tree led to identification of the appropriate emission estimations and/or modules in the ESD matrix.

The *target funnel* methodology has been structured in such a way that in future work, it can easily be implemented into a computer program. The first results are satisfactory indicating the usefulness of this approach.

However, additional work is needed in order to exploit the tool in a more comprehensive way for REACH. For example, there is no complete matrix of industrial activities, processes, and emission scenarios are yet available. In addition, the present lists of ICs and UCs in the TGD need further development and, the current ESDs are mutually quite different of structure and scope making the routing through the decision tree difficult.

As regards future research, it is recommended to firstly analyse the available ESDs in order to harmonize structures facilitating the selection of appropriate identifiers for the decision tree.

6 Stand-alone emission estimation tools

The registrant under REACH needs to base his quantification related to emissions from down stream uses on assumptions since he usually does not know the details of the condition of use. Five types of quantification are needed to derive exposure estimates and subsequent risk characterisation as required for the registrant's chemical safety assessment under REACH.

- The volume of substance applied downstream will often be broad default values applied for more than one sector, process or product group. The registrant will communicate the dependency of exposure related to the applied substance volume.
- The same applies for locally available volume of the receiving environments, e.g. river water flow or indoor air exchange.
- The emission factor driven by process or product specific parameters is the core information to be obtained from a sector or branch specific library or directly from the customers or their organisation. This emission factor may already include process or

management integrated pollution prevention measures. A separate quantification of the risk management efficacy may be difficult.

- The type and efficacy of additional risk management measures (onsite abatement or external abatement like municipal waste water treatment) and the parameters driving the efficacy (e.g. substance properties) is the fourth quantification to be made.

- The annual emissions from a site may be distributed over a specific number of days in the year. Hence the number of release-days is an additional information relevant for the registrant.

The information should reflect the typical conditions in the respective market. Hence neither worst case assumptions nor the assumption that all companies do apply best practise or best available technique would lead too an adequate safety assessment.

In order to make existing sector specific information on releases to the environment better accessible one of the OECD Emission Scenario Documents has been transformed into a web based IT tool. A second ESD was used for testing the adaptation of the tool to the conditions in other industry branches. The tool is called ***Emission Estimation Tool (EET).***

The emission estimation tool integrates various single emission estimation modules. In a library it would be identified by the IC and the type of chemical product (preparations) typically used in this sector. All other identifiers (e.g. life cycle stage, type of processing, substance function, size of source, exposure pathways) are integrated in the tool itself.

Branch-specific determinants of emissions can probably be understood as modulations of these five generic emission drivers defined above. In this case, it should be possible to use the following generic formula as a starting point for emission estimation:

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

E	emission rate [kg.d^{-1}]
$Q_{product}$	the quantity of substance, preparation or article processed or used per time period at a site or in a region [kg.yr^{-1}]
$C_{chemical}$	the concentration of the chemical in the product [kg.kg^{-1}]
F_x	relevant emission factor [-]
$F_{abatement}$	efficacy factor(s) for one or more abatement technique(s) (= Risk Management Measures) [-]
$T_{emission}$	the emission period [d.yr-1]

Usually not all emissions from a process, a product or a sector are caught by additive abatement techniques. Thus, the resulting emission rate is not only driven by the technical efficacy of a measure if applied but also by the degree to which emissions are caught by the respective additional abatement technique.

6.1 Emission estimation tool for plastic additives

The tool has been developed based on the OECD ESD on plastic additives (OECD ESD No. 3, 2004) covering ten EEMs. The main elements of the EET are (for more details please see Annex 3):

- Guided step by step emission estimates (to air, water, soil, waste) for each of the 5 main life cycle stage of a substance used in plastic compounds (synthesis, compounding, conversion, service life, waste treatment).

- The tool can be applied by manufacturers, importers, compounders and converters for their own processes and for the processes of their customers. The web application does not allow yet to store the (unspecific) data-sets from iteration level 1 and 2, e.g. derived from the tentative exposure scenario, or an incomplete dataset beyond the actual log-in time and to send it for completion or revision to the customers. However, the final results can be printed at the end.

- A local and a regional scenario are needed to assess service life and waste treatment, however only two of the four scenarios available in the tool yet (regional service life and local waste treatment)

- Seven parameters determine the release per day/year:

    - Used amount in registrant's own process and at largest customer (compounder) respective customer of customer (converter) per time;

    - Broad type of additive and corresponding releases;

    - Substance properties, including level of dustiness;

    - Processing type and processing temperature;

    - Indoor or outdoor service life;

    - Fraction to external waste water or waste treatment and efficacy of this treatment;

    - Fraction to onsite abatement and efficiency of onsite abatement.

- Three levels of iteration can be performed at each life cycle stage:

    - Level 1: Automated default setting only driven by substance amount (registrant's volume or DUs volume[9] and estimate of total EU market volume) and substance properties. All other determinants of release and exposure are based on the TGD (fraction main source, release days and emission factor for M/I stage) and ESD's reasonable worst case scenario for plastic additives (emission factors). No risk management measures are regarded to be in place.

9 The most upstream applicant of the tool inserts the annual volume handled by his company.

- Level 2: Iteration level 2 is based on pick-lists related to release days, fraction of main source, additive types and corresponding fraction of release, process/article types and corresponding fraction of release; the fraction through STP and the locally available volume of the receiving compartment are specified in free text mode.

- Level 3: Iteration level 3 is based on free text related to release days and processed amount per day, losses from process (resulting from specific process design and integrated measures), fraction to on-site abatement, efficiency of onsite abatement.

- Simple fate and exposure estimates for the water pathway (reduced version of the Simple-Treat model) are integrated in the tool in order to illustrate how iteration will be carried out, once the EEMs are connected to an exposure assessment and risk characterisation module.

The tool can be tried out under http://www.emisiontool.com. A flyer and a presentation explaining the tool are attached in Annex 4.

6.2 Emission estimation tool for photo-chemicals

The generic approach of the emission estimation tool has been tested in a second supply chain (photo-chemicals, industrial category 10). The related ESD (OECD ESD No. 5, 2004) describes emissions during industrial use (of processing solutions and photographic materials) and during waste disposal of used processing baths. Three different emission estimation modules (EEMs) have been identified and located in the corresponding cells of the ESD matrix.

In the following step, one EEM (No. 10.1 “Release of photo-chemicals from the industrial or professional use of processing solutions”) has been transformed into the emission estimation tool. During this work it has been analysed whether the principles and the IT-structure used for plastic additives could be used as a “blue print” for the second supply chain. This analysis led to the following conclusions:

The main structural elements of the plastic additives IT tool support and facilitate the generation of the module for the photo-chemicals. These elements can be used in the same way in both supply chains:

- differentiation between basic information (e.g. substance inherent properties, EU market volume, manufacturers/importers volume, fraction of main source and release days) and life cycle specific information (e.g. area of processed material and carry over rate of processing chemicals in multi-stage industrial processes, impacts of process temperature on emission rates)

- “horizontal” differentiation between five life cycle stages, however with the difference that i) releases from article service life is not relevant for photo-chemicals, ii) private use of photo-chemicals may be relevant in addition to industrial use and professional use and iii) recovery/recycling is relevant for photo-chemicals, compared to plastic additives where the plastic matrix is the target for recycling

- “vertical” differentiation between three iterations levels
- application of the generic formula for a) emission estimation and b) assessment of the risk to the aquatic environment

The identifiers “industry category”, “life cycle stage”, “type of chemical product”, “technical function of a substance”, “type of process” and “size of source” are relevant in both supply chains – with three major differences:

- Identifier “technical function”: This identifier has been much deeper differentiated in the plastic additive ESD (21 different types of plastic additives with different emission factors) than in the ESD of photo-chemicals (15 different functions driving the concentration in the bath; only 3 function-specific emission factors).
- Identifier “type of process”: The process type is the most important identifier in the ESD on photo-chemicals. Three different process types are addressed here. For each of this process types (“bath type A, B or C”) a specific formula for the emission estimation is given. The range of emission factors to waste water cover 10% to 100% of substances applied. The ESD on plastic additives is more specific on process types: 11 different processes at converter’s level are specified with their default emission factors to waste water (ranging from 0.001% to 2.5%), air and waste, however all refer to the same formula.
- Identifier “size of sources”: The ESD on photo-chemicals contains detailed information on several point sources (whole sale finisher, professional lab and others) with the related figures on amount of processed photographic material per year. This value in combination with a standard concentration of substance in the bath is used to determine the substance input potentially emitted to the environment. In comparison to that, the B tables of the TGD usually provide the fraction of the main source as a substance related input value and do not refer to the amount of (photographic) material processed per time unit. Also the ESD on plastic additives makes no reference to plastic material processed at conversion stage.

For the calculation of the emission the same basic formula can be used in the first iteration. In the second and third iteration three major differences occur in the life cycle step “industrial use” for photo-chemicals:

- The amount of photographic material processed per day ($Area_{mat}$) is used in the calculation – in combination with figures on concentrations of substances in the processing baths. In the case of plastic additives, the amount of the substance used by the main client (Q_{own} x $f_{mainsource}$) has been used instead of an area-related parameter (except for the formulation stage).
- No emission factors from process before abatement are presented in the ESD (in opposite to the ESD on plastic additives). Instead of this, the fraction of the substance which is released is calculated using process-specific parameters typical for developing processes (carry over rates (CO rates) and replenishing rates (RR)), including integrated risk management measures. Values for these parameters are given in the ESD

and can be translated into a pick-list, like the factors driving the emission in the tool on plastic additives.

- The influence of the process-specific parameters on the emission depends on the bath-type (baths with or without direct discharge to wastewater, baths with processing/recovery of the solutions after use). Therefore in the ESD three different (but similar structure) formulas for the emission estimation have been proposed. This is in principal an integration of the abatement factor (or risk management step) into the primary emission factor. Since the measures are process integrated, it would not have been useful to define an emission factor reflecting the process technique in the past and a factor reflecting the abatement efficacy of integrated process techniques.

These differences required adaptations of the basic formula and some modifications during the development of the stand-alone-IT tool for the photo-chemicals. It was in particular necessary to convert the “carry-over-rate” and “replenishing rate” into the generic emission factor of the formula. Also an algorithm was needed to covert “processed material” and “bath concentration” into the Q-term of the generic formula. However, in principal it would have been also possible to recalculate these values into the term “fraction of main source” to make it compatible to the B-Table approach. In this case, the values for the “fraction of main source” would be determined by the bath type and substance function. Beside this, no changes in the frame of the IT tool and its basic elements have been necessary.

Hence, it was possible to use the same generic approach in the second supply chain. The resources needed for the life cycle stage “industrial use” sum up to:

- Approximately 25 consultant days were spent for the analysis of the ESD on photo-chemicals, the exchange with the stakeholders in the photochemical supply chain and the translation of the information into a ready-to-use document for the IT tool development. The 25 man-days do not include the stakeholders’ resources spent in the consultation process.
- The IT tool adaptation for the module was approximately 10 additional days.

Having laid the conceptual basis, further modules can now be integrated with limited effort regarding IT-development (e.g. 10 days per ESD), once the IT-development document for a specific branch/supply chain has been defined.

7 Conclusions and recommendations

7.1 Conclusions

The *Matrix Project* has generated three major outcomes. Firstly, a **Matrix** provides an overview which *Emission Estimation Modules* (EEMs) are available in the EU TGD and OECD Emission Scenario Documents and can be used for environmental exposure assessment under REACH. Also, a number of ESDs have been analysed in depth in order to identify structural similarities and differences in the current documents. Secondly, a **Target Funnel** was conceptualised as a tool to identify suitable EEMs for a certain use (or a group of uses) of a substance. Thirdly, the OECD ESD on plastic additives has been transformed into a **stand-alone**

IT-Tool (including a manual) for emission estimation under REACH (**REACH EET**), implemented as a web application. The IT-tool structure as developed for additives in plastic has also been applied to **photo-chemicals** in order to test the feasibility of a generic approach.

From the three components of the *Matrix Project*, a number of general conclusions can be drawn:

7.1.1 For quite a number of industrial uses of substances environmental emission estimation is possible based on the available OECD documents and the TGD. 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* and *the target funnel* developed in the current project are relevant steps in making this information better accessible.

7.1.2 The current categorising approaches related to uses of substances (based on IC/UC-combinations) are not sufficiently connected with the emission patterns driven by the type of application process (in combination with the type of chemical product in which the substance under assessment is contained).

7.1.3 Transforming an ESD into an IT tool based on a generic structure and emission estimation formula makes the information useful under REACH and facilitates the revisions and adaptations of ESDs needed to fit into the REACH concept. Due to the variety of approaches in the ESDs, the transformation consumes significant resources (about 35 to 50 consultant and IT-developer-days per ESD), even when a generic IT framework is available.

7.1.4 Although a generic structure seems feasible in most cases, the flexibility of the EET prototype allows adaptations to the particular conditions of use in certain supply chains or a certain market. Also, emission estimation modules being of relevance across various sectors of industry can be incorporated into the EET. Both approaches can be run in parallel, sectors or branch specific EETs integrating a number of EEMs and cross cutting EEMs useful for emission estimation across various sectors.

7.1.5 The EET supports Exposure Scenario development under REACH by less experienced safety assessors due to the systematic and guided process from less specific information to more specific information.

7.1.6 An IT supported tool to identify suitable EEMs (once a tentative Exposure Scenario has been defined by an actor in the supply chain) is crucial for efficient work under REACH. The *Target Funnel* is a first generic approach proposed for such a tool. It would be essential that the system of short titles for uses and exposure scenarios needed under REACH and the identifiers in a library of EEMs fit together. Such a common navigation system is needed to link the Exposure Scenarios under REACH to tools for quantification of environmental releases.

7.1.7 A set of 7 to 10 identifiers for EEMs has been defined in the current project. Also options to cluster uses under certain standard EMMs have been theoretically explored. However, clustering is only possible once the most relevant processes leading to emissions have been described in a standard structure and language following e.g. the *matrix* approach.

7.1.8 Major conceptual gaps in emission estimation still exist related to the waste life stage of substances. With regard to service life, however, the ESD on plastic additives can be used as a starting point to further develop the concept to assess releases from articles during service life.

7.1.9 It is not always possible to specify the efficacy of pollution prevention technique integrated into the manufacturing process itself. Under REACH this may lead to a situation that a use even without any additional risk management measures can be regarded safe and hence traditional risk management measures do not occur in the exposure scenario.

7.2 Recommendations

Based on these conclusions, the project group has worked out a number of recommendations for further work, in particular with regard to the technical implementation of REACH.

7.2.1 Recommendation related to further ESD development

There is a clear need to fill gaps and to update or refine the emission estimation modules currently available. Regarding industrial use, consumer use and product service life this should be seen as task of industry, since the responsibility to come up with valid safety assessment is on them. However, there are processes and risk management measures outside the control of substance manufacturers, down stream users and producers of articles, like e.g. waste and waste water treatment. Here public authorities should possibly take the lead in developing emission estimation modules.

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. 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 generic scenarios of the US EPA Office of Pollution, Prevention and Toxics (OPPT)

In each ESD or the documentation for newly developed ESDs a table should be included indicating each emission estimation module together with ICs, UCs, MCs, process types, product types and RMMs which have been taken into consideration. Also, a mini-matrix should be used to indicate which life cycle stages and which environmental compartments are addressed by the EEMs. This would allow labelling the EEMs with a set of identifiers in an electronic library.

Newly identified emission estimation modules, suitable to meet the REACH requirements, should be allocated to the electronic library based on the ESD matrix. The matrix can serve as a reference point for the selection of appropriate data sets for emission estimation.

Risk management measures should be addressed, whenever an EEM is newly developed or refined. A list of standard techniques including default values for efficacy would be a very useful instrument. However, some risk management measures are integral part of process design and process management. Such cases, where the emission factor already reflects part of the risk management should be clearly flagged in the ESDs.

Also data on the emission pattern in space and time (duration, frequency, special distribution, emissions during service life) should be part of ESDs or emission estimation modules in future.

7.2.2 Recommendations related to REACH implementation projects

The current industrial category "Others" (IC 0/15) should be further diversified since many industrial applications do not fit into the current ICs.[10] This could be done under the umbrella of the RIP 3.2-2 process.

The existing data on emissions of chemicals 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. Whether this is a large library or whether it has the form of an EET as developed for plastic additives could be left open for the time being. Additive measures suitable to ensure safe use can be selected from this system. In any case, the system of identifiers for EEMs should be further developed, including an IT - navigation system to identify the suitable EEM. The *target funnel* can be used as a starting point here.

7.2.3 Recommendations for further EET development

First of all, the EET for plastic additives in its current stage is not linked to the exposure models currently used in the EU. However, a linkage of the EET to other IT tools on fate and distribution requires the agreement on such tools for REACH. Then, interfaces (e.g. to EUSES or SimpleTreat or other tools) may be defined. Hence it would be worthwhile to discuss conceptually how this link could look like. As long as this is not available, the current tool or other emission estimation tools can be used for demonstration purposes only since the sediment, the soil and the biota compartment cannot be assessed.

Also, the tool has still a number of systematic limitations that should be removed in a follow-up project, taking into account also the outcome of the further work under RIP 3.2-2.

- The first iteration level is overly conservative due to the assumption that a manufacturer of a substance sells his whole production volume to one customer-site and no risk management measures would be in place at all.
- If the formulator or the industrial users starts the assessment based on his own volume of substance used it is not possible to automatically skip the first iteration level (which typically reflects the assessment perspective of the substance producer).
- The local scenario for the service life stage and the regional scenario for the waste life stage are still missing.
- Only one waste disposal operation (local scenario for a non-standard landfill) is yet included in the tool.
- Abrasive conditions during service life are not yet well reflected in the emission factor for service life.
- There is no pick-list yet for abatement measures typical in the sector.
- REACH does not require the registrant to take into account any background emissions from sources not related to his production processes, production volume and his market. It

[10] See also report by Bjorn Hansen and Johan Verburgh (1997): Overview of Industrial and Use Categories for EU H(L)PVCs.

is not yet clear who will generate this information and which role it may play in substance evaluations under REACH. Nevertheless the tool allows to calculate background emissions based on the EU market volume. However, the regional background emission cannot be iterated yet, it is fixed based on very rough assumptions.

- Options like SAVE, EXPORT or PRINT have still to be included or enlarged.

Most of these limitations could be removed with some investments into further IT development of a more sophisticated control logic. This should address the following issues:

- Support for decision-making, i.e. for a choice of different calculations to be performed within one module. So far only a variety of factors or parameters can be selected for use in <u>one</u> calculation.
- Adaptation of the user-interface to support user-friendly handling of multiple decision-making.
- Support for different scenarios to be run alternatively within one module: Currently only <u>one</u> calculation is possible for any module. The choice among different scenarios within one module would facilitate for example
    - to calculate different product types within the service life stage
    - to calculate different disposal techniques in the waste stage
    - to sum up exposure values of different scenarios for a given stage
- Consolidation of all calculations performed as a downloadable PDF (Adobe Acrobat document)

The software application itself would benefit substantially from

- implementing a user management and storage of user data: Currently, data storage is not supported, since there is no user management powered by a database backend. Therefore, in the current version, all user data are lost when disconnecting from the website or when switching from one supply chain (e.g. plastic additives) to another one (e.g. photo-chemicals).
- improvement of the administration of control data: For example, some control data are identical across supply chains, which means they are redundant. This can easily lead to errors and should be avoided by supporting concurrent use of control data across supply chains.

The IT tool for plastic additives has not yet been systematically validated based on available EU risk assessments for plastic additives (e.g. plasticisers and flame retardant). This should be one of the first tasks in the follow-up project.

The stand-alone IT tool for plastic additives and the module for photo-chemicals should be tried out by a larger number of users before further work is invested[11]. Special attention should be given to the question whether this tool is suitable for day by day routine work or whether it is rather a training tool. Possibly the more experienced user would prefer a simple spread-sheet with a set of pick-lists.

In general, an EET should be understood as a “living” tool which allows to adapt and revise assumptions depending on the consultation process in the corresponding supply chains or branches.

A successful “translation” of the emission scenario documents into branch-specific support tools needs close cooperation with the actors of the supply chain. This has been a crucial element in the Matrix project for both supply chains.

[11] The exemplification of Exposure Scenarios in the RIP 3.2-2 process (REACH Implementation Project on CSA/CSA as part of the EU Commission’s Interim Strategy) may be an opportunity to test the tool.

Annex 1: The ESD Matrix

Results of part B1 of the OECD Matrix Project

This matrix shows for each industrial category, which A- and B-tables of the EU 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 emission estimation module as well as the reference are provided as foot notes.

For further information see the detailed reports of the project parts A, B1, and B2.

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March 2006

Introduction to the use of the ESD Matrix

The following matrix has been developed in the framework of the OECD Matrix Project. The aim of the OECD Matrix Project is to support the use of already-existing emission estimation data for the exposure assessment which is required under REACH. The results of the project are documented in the Matrix Summary Report with six supplements.

Within the EU TGD (Technical Guidance Document on Risk Assessment) and the OECD emission scenario documents, a large amount of branch-specific emission data has been published. These data can be a valuable starting point for the exposure assessment which is required under REACH. Unfortunately, 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.

The ESD Matrix aims to give an overview, which data sets referring to emission estimation are available in the TGD and the OECD emission scenario documents. In order to simplify the use of these documents, the information in OECD Emission Scenario Documents has been unitised into smaller data sets called "Emission Estimation Modules (EEM)". Each Emission Estimation Module refers to a specific emission situation.

In order to structure the matrix, the system of industrial categories of the TGD is used. It distinguishes between 15 industrial categories. As a second structural element, eight life cycle stages are used.

For each industrial category (e.g. IC 7, Leather processing industry), the corresponding first two lines of the Matrix indicate in which tables of the TGD information on release factors (A-table), on the size of a local source and on the number of release days (B-table) can be found. (The A-tables of the EU TGD contain release factors for 16 industrial categories regarding the different life cycle stages. 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.)

For a number of industrial branches additional information is available from OECD emission scenario documents. If this is the case, it is indicated in the third line of the matrix part. A short description of the module as well as the reference are provided.

In order to use the matrix, it should be identified in a first step which industrial categories are of relevance for the final use of a substance (as such, in a preparation or an article). In a second step it should be clarified which life cycle steps are of importance.

For further information regarding the use of the ESD matrix and the selection of the appropriate emission estimation module, see the Matrix Summary Report and its supplements.

Annex 1: The ESD Matrix

IC	Allocation of A- and B-tables, EE Modules, and References	Production				Formulation			Industrial use		Prof. use	Private use		Service life	Re-covery	Waste disposal	TGD ESD and others		OECD ESD	
1	**Agricultural industry**																			
	A-tables	A1.1				A2.1			A3.1											
	B-tables	B1.1	B1.2	B1.3	B1.4	B2.1	B2.2	B2.3	B3.1											
	EE Modules																			
2	**Chem. industry: basic chemicals**																			
	A-tables	A1.1				A2.1			A3.2											
	B-tables	B1.1	B1.5			B2.5	B2.4		B3.2											
	EE Modules																			
3	**Chem. industry: chemicals used in synthesis**																T_E 3[1]			
	A-tables	A1.1	A1.2			A2.1			A3.3											
	B-tables	B1.2	B1.6			B2.3	B2.4		B3.2											
	EE Modules																			
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								EEM 4.1[2] EEM 4.3[5]	EEM 4.2[3] EEM 4.4 / 4.5[6]									OECD _9[4]	
5	**Personal/domestic**																T_E 5[7]			
	A-tables	A1.1	A1#			A2.1	A2#					A4.1								
	B-tables	B1.6	B1.7			B2.1	B2.3					B4.1	B4#							
	EE Modules																			
6	**Public domain**																T_E 6[8]			
	A-tables	A1.1	A1#			A2.1	A2#		A3.5											
	B-tables	B1.6	B1.7			B2.1	B2.3		B3.3											
	EE Modules																			
7	**Leather processing industry**																T_E 7[9]			
	A-tables	A1.1	A1.3			A2.1			A3.6											

IC	Allocation of A- and B-tables, EE Modules, and References	Production				Formulation			Industrial use		Prof. use	Private use		Service life	Re-covery	Waste disposal	TGD ESD and others		OECD ESD	
		or																		
	B-tables	B1.4	B1.8	B1.9		B2.6	B2.3	B2.4	B3.4											
	EE Modules								EEM 7.1[10]										OECD _8[11]	
8	**Metal extraction industry, refining and processing industry**																T_E_8[12]			
	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[13]										OECD _10[14]	OECD_12[15]
	EE Modules, Lubricants					EEM 8.2[16]						EEM 8.3							OECD _10[17]	
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	B2.7	B2.8	B3.7			B4.1								
	EE Modules																			
10	**Photographic industry**																T_E_10[18]			
	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[19]	EEM 10.2[20]					EEM 10.3[21]				OECD _5[22]	
11	**Polymers industry**																T_E_16R[23]			
	A-tables	A1.1				A2.1			A3.10	A.3.11										
	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[24] EEM 11.3[31]	EEM 11.2[25] EEM 11.4[32]		EEM 11.5[26]	EEM 11.6[27]				EEM 11.7[28] EEM 11.8[33]		EEM 11.9[29] EEM 11.10[34]			OECD _3[30]	
	EE Modules, Rubber Additives					EEM 11.R.1[35]	EEM 11.R.2[36]		EEM 11.R.1[37]	EEM 11.R.2[38]				EEM 11.R.3[39]					OECD _6[40]	
12	**Pulp, paper, and board industry**																T_E_12[41]			
	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				

IC	Allocation of A- and B-tables, EE Modules, and References	Production				Formulation			Industrial use		Prof. use	Private use		Service life	Re-covery	Waste disposal	TGD ESD and others		OECD ESD	
	EE Modules																		OECD _	
13	**Textile processing industry**																T_E_13[42]			
	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[43] EEM 13.3[47]	EEM 13.2[44] EEM 13.4[48]				EEM 13.5[45]					OECD _7[46]	
14	**Paints, lacquers, and varnishes industry**																T_E_14[49]			
	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					EEM 14.1-9[50]			EEM 14.10 -23.[51]			EEM 14.12[52]		EEM 14.10-23[50]		EEM 14.1-23[50,51], 14.24[53]			OECD _20[54]	
	EE Modules, Automotive coating[1]								EEM 14.A1-A6[55]											
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.																		OECD _11[56]	
0/ 15	**Others**																T_E-16_R[57]			
	A-tables	A1.1				A2.1			A3.16											
	B-tables	B1.2	B1.6			B2.3	B2.8		B3.14			B4.5				B5.3				
	EE Modules																			

[1] The Emission Estimation Modules (EEMs) regarding automotive coating can be related to industrial category 14 as well as to industrial category 16.

[1] T_E_3: IC 3: Emission scenario document “Chemical Industry: chemicals used in synthesis”, TGD 2003, chapter 7, part IV.

[2] **EE module IC 4.1:** Emission scenario for release of photoresist from transport container residues. Emission collected as waste (OECD ESD No. 9, 2004/D9, p. 13).

[3] **EE module IC 4.2:** Emission scenario for release of photoresist from equipment cleaning. Emission collected as waste (OECD ESD No. 9, 2004/D9, p. 13).

[4] OECD 2004/D9: OECD Series on Emission Scenario Documents, No. 9, Emission scenario document on photoresist use in semiconductor manufacturing. OECD, Environment Directorate, June 2004.

[5] **EE module IC 4.3:** Emission scenario for release of photoresist from dispensed photoresist. Emission to waste (OECD ESD No. 9, 2004/D9, p. 14).

[6] **EE module IC 4.4:** Emission scenario for release of photoresist from developing the wafer. Emission collected as waste water (OECD ESD No. 9, 2004/D9, p. 15).

EE module IC 4.5: Emission scenario for release of photoresist from etching and stripping of wafer. Emission collected as waste (OECD ESD No. 9, 2004/D9, p. 15).

[7] T_E_5: IC-5,6 Emission scenario document “Personal/Domestic and Public domain”, TGD 2003, chapter 7, part IV.

[8] T_E_5: IC-5,6 Emission scenario document “Personal/Domestic and Public domain”, TGD 2003, chapter 7, part IV.

[9] T_E_7: IC-7 Emission scenario document “Leather processing industry”, TGD 2003, chapter 7, part IV.

[10] **EE module IC 7.1:** Emission scenario for release of chemicals used in leather processing. Emission to waste water (OECD ESD No. 8, 2004/D8, p. 27).

[11] OECD 2004/D8: OECD Series on Emission Scenario Documents, No. 8, Emission scenario document on leather processing. OECD, Environment Directorate, June 2004.

[12] T_E_8: IC-8 Emission scenario document “Metal extraction industry, refining and processing industry”, TGD 2003, chapter 7, part IV**.**

[13] **EE module IC 8.1:** Release of a water-miscible cooling lubricant emulsion in the watery phase during waste / recovery treatment (Baumann, 1999, p. 15 – 17).

[14] OECD 2004/D10: OECD Series on Emission Scenario Documents, No. 10, Emission scenario document on lubricants and lubricant additives. OECD, Environment Directorate, November 2004.

[15] OECD 2004/D12: OECD Series on Emission Scenario Documents, No. 12, Emission scenario document on metal finishing. OECD, Environment Directorate, November 2004.

[16] **EE module IC 8.2:** Release of an aquaeous cooling lubricant solution in the watery phase during waste / recovery treatment (Baumann, 1999, p. 19).

[17] OECD 2004/D10: OECD Series on Emission Scenario Documents, No. 10, Emission scenario document on lubricants and lubricant additives. OECD, Environment Directorate, November 2004.

[18] T_E_10: IC-10 Emission scenario document “Photographic industry”, TGD 2003, chapter 7, part IV.

[19] **EE module IC 10.1:** Release of photochemicals by the use of processing solutions (OECD ESD No. 5, 2004/D3, p. 11 – 21).

[20] **EE module IC 10.2:** Release of ingredients of the emulsion layer of the photographic material during processing. (OECD ESD No. 5, 2004/D3, p. 25 – 26).

[21] **EE module IC 10.3:** Release of photochemicals during waste disposal of used processing baths by specialised disposal companies (OECD ESD No. 5, 2004/D3, p. 22-25).

[22] OECD 2004/D3: OECD Series on Emission Scenario Documents, No. 5, Emission Scenario Document on Photographic Industry. OECD, Environment Directorate, June 2004.

[23] T_E_16: IC-16 Emission scenario document “Others: Rubber industry”, TGD 2003, chapter 7, part IV.

[24] **EE module IC 11.1:** Release of additives from materials handling to water (OECD ESD No. 3, 2004/D4, p. 32).

[25] **EE module IC 11.2:** Release of additives from materials handling to air (OECD ESD No. 3, 2004/D4, p. 32).

[26] **EE module IC 11.5:** Release of additives from conversion to water (OECD ESD No. 3, 2004/D4, p. 32).

[27] **EE module IC 11.6:** Release of additives from conversion to air (OECD ESD No. 3, 2004/D4, p. 32).

[28] **EE module IC 11.7:** Release of additives during the service life of polymers to water (OECD ESD No. 3, 2004/D4, p. 35).

[29] **EE module IC 11.9:** Release of additives during the service life of polymers to air (OECD 2004/D4, p. 35).

[30] OECD 2004/D4: OECD Series on Emission Scenario Documents, No. 3, Emission Scenario Document on Plastics Additives. OECD, Environment Directorate, June 2004.

[31] **EE module IC 11.3:** Release of additives from compounding to water (OECD ESD No. 3, 2004/D4, p. 32).

[32] **EE module IC 11.4**: Release of additives from compounding to air (OECD ESD No. 3, 2004/D4, p. 32).

[33] **EE module IC 11.8:** Release of additives during the service life of polymers to air (OECD ESD No. 3, 2004/D4, p. 35).

[34] **EE module IC 11.10:** Release of additives from disposal of a polymer product, to water (OECD 2004/D4, p.36).

[35] **EE module IC 11R.1:** Emission scenario for release of additives during formulation / processing of rubber. Emission to waste water (OECD ESD No. 6, 2004/D7, p. 25).

[36] **EE module IC 11R.2:** Emission scenario for release of additives during formulation / processing of rubber. Emission to air and soil (OECD ESD No. 6, 2004/D7, p. 30 et sqq.).

[37] **EE module IC 11R.1:** Emission scenario for release of additives during formulation / processing of rubber. Emission to waste water (OECD ESD No. 6, 2004/D7, p. 25).

[38] **EE module IC 11R.2:** Emission scenario for release of additives during formulation / processing of rubber. Emission to air and soil (OECD ESD No. 6, 2004/D7, p. 30 et sqq.).

[39] **EE module IC 11R.3:** Emission scenario for release of rubber additive breakdown production by abrasion of tyres. Emission to soil (OECD ESD No. 6, 2004/D7, p. 31 et sqq.).

[40] OECD 2004/D7: OECD Series on Emission Scenario Documents, No. 6, Emission scenario document on additives in rubber industry. OECD, Environment Directorate, June 2004.

[41] T_E_12: IC-12 Emission scenario document “Pulp, paper and board industry”, TGD 2003, chapter 7, part IV.

[42] T_E_13: IC-13 Emission scenario document “Textile processing industry”, TGD 2003, chapter 7, part IV.

[43] **EE module IC 13.1:** Local emission of substances emitted in pre-treatment processes (preparation agents, sizing agents, biozides; from imported fabrics/fibres). Emissions to water. Daily emission rates (OECD ESD No. 7, 2004/D5, chap. 10.1.1, p. 49).

[44] **EE module IC 13.2:** Local emission of substances emitted in exhaust processes (basic chemicals, dyestuffs, auxiliaries). Emissions to water. Daily emission rates (OECD ESD No. 7, 2004/D5, chap. 10.1.2, p. 50).

[45] **EE module IC 13.5:** Continental/regional emission of substances from articles during their service life. Emissions to water. Yearly emission rates (OECD ESD No. 7, 2004/D5, chap. 10.3, OECD 2004/D5, p. 55).

[46] OECD 2004/D5: OECD Series on Emission Scenario Documents, No. 7, Emission Scenario Document on Textile Finishing Industry. OECD, Environment Directorate, June 2004.

[47] **EE module IC 13.3:** Local emission of substances emitted in padding processes, printing and coating (basic chemicals, dyestuffs, auxiliaries). Emissions to water. Daily emission rates (OECD ESD No. 7, 2004/D5, chap. 10.1.3, p. 51).

[48] **EE module IC 13.4:** Local emission of substances emitted in the off-gas of finishing recipes (from a stenter) and emissions of preparation agents. Emissions to air. Daily emission rates (OECD ESD No. 7, 2004/D5, chap. 10.2, p. 52).

[49] T_E_14: IC-14 Emission scenario document “Paints, lacquers and varnishes industry”, TGD 2003, chapter 7, part IV.

[50] **EE module IC 14.1:** Emission calculation (release factors) for formulation of organic solvent-borne coatings, standard batch. Emission to air, water and waste (RPA 2003, p.35 et sqq., table 4.3, p. 42).

EE module IC 14.2: Emission calculation (release factors) for formulation of organic solvent-borne coatings, large batch (10.000 l). Emission to air, water and waste (RPA 2003, p.44 et sqq., table 4.6, p. 46).

EE module IC 14.3: Emission calculation (release factors) for formulation of water-borne, aqueous dispersion coatings, standard batch. Air, water and waste (RPA 2003, p.51 et sqq., table 5.6, p. 54).

EE module IC 14.4: Emission calculation (release factors) for formulation of water-borne, aqueous dispersion coatings, large batch. Air, water and waste (RPA 2003, p.56 et sqq., table 5.9, p. 57).

EE module IC 14.5: Emission calculation (release factors) for formulation of water-borne, water-reducible coatings and colloidal dispersions, standard batch. Air, water and waste (RPA 2003, p.58 et sqq., table 5.12, p. 61).

EE module IC 14.6: Emission calculation (release factors) for formulation of water-borne, water-reducible coatings and colloidal dispersions, large batch. Air, water and waste (RPA 2003, p.62 et sqq., table 5.15, p. 63).

EE module IC 14.7: Emission calculation (release factors) for formulation of melt-blend powder coatings, standard batch. Air, water and waste (RPA 2003, p.67 et sqq., table 6.1, p. 71)

EE module IC 14.8: Emission calculation (release factors) for formulation of melt-blend powder coatings, large batch. Air, water and waste (RPA 2003, p.75 et sqq., table 6.5, p. 76).

EE module IC 14.9: Emission calculation (release factors) for formulation of dry-blend powder coatings, standard batch. Air, water and waste (RPA 2003, p.79 et sqq., table 6.7, p. 82).

51 **EE module IC 14.10:** Emission estimate for application of wooden furniture coatings, spray application (RPA 2003, p.94 et sqq., fig. 3.1, p. 97).

EE module IC 14.11: Emission estimate for application of wooden furniture coatings, flat line application (RPA 2003, fig. 3.2, p. 99).

EE module IC 14.12: Emission estimate for application of decorative paints, general public use (RPA 2003, fig. 4.1, p. 104).

EE module IC 14.13: Emission estimate for application of decorative paints, professional use (RPA 2003, fig. 4.1, p. 104).

EE module IC 14.14: Emission estimate for application in automotive coating, original automotive equipment manufacture (OEM), (RPA 2003, fig. 5.2, p. 114).

EE module IC 14.15: Emission estimate for application in automotive coating, refinishing, dry back booth (RPA 2003, fig. 5.3, p. 115).

EE module IC 14.16: Emission estimate for application in automotive coating, refinishing, wet back booth (RPA 2003, fig. 5.4, p. 116).

EE module IC 14.17: Emission estimate for application of metal packaging coatings, 2-piece-beer/beverage can, external coating (RPA 2003, fig. 6.3, p. 123).

EE module IC 14.18: Emission estimate for application of metal packaging coatings, 2-piece-beer/beverage can, internal lacquering (RPA 2003, fig. 6.4, p. 123).

EE module IC 14.19: Emission estimate for application of metal packaging coatings, 3-piece-food/ general line can (RPA 2003, fig. 6.5, p. 124).

EE module IC 14.20: Emission estimate for application of coil coatings (RPA 2003, fig. 7.2, p. 130).

EE module IC 14.21: Emission estimate for application of marine coatings (non-antifoulant) (RPA 2003, fig. 8.1, p. 135).

EE module IC 14.22: Emission estimate for application of coatings for aircrafts painting (RPA 2003, fig. 9.1, p. 140).

EE module IC 14.23: Emission estimate for application of coatings for rail vehicle painting (RPA 2003, fig. 10.2, p. 146).

52 **EE module IC 14.12:** Emission estimate for application of decorative paints, general public use (RPA, 2003/D6, fig. 4.1, p. 104).

53 **EE module IC 14.24:** Emission estimate for the treatment of coatings wastes (RPA 2003, fig. 11.2, p. 150).

54 OECD 2003/D6: RPA (Risk&Policy Analysts Limited); Emission Scenario Document Chemicals used in the coatings industry: paints, lacquers and varnishes. Draft, June 2003. OECD.

55 **EE module IC 14A.1:** Emission scenario for release of coatings by spray-application from captured overspray. Emission collected as waste (OECD ESD No. 11, 2004/D 11, p.19).

EE module IC 14A.2: Emission scenario for release of coatings by spray-application from gun cleaning. Emission collected as waste (OECD ESD No. 11, 2004/D 11, p.19).

EE module IC 14A.3: Emission scenario for release of coatings by spray-application from container residue. Emission collected as waste (OECD ESD No. 11, 2004/D 11, p.20).

EE module IC 14A.4: Emission scenario for release of coatings by spray-application from overspray. Emission to air (OECD ESD No. 11, 2004/D 11, p.21).

EE module IC 14A.5: Emission scenario for release of coatings by spray-application from clean-up of mixing apparatus and guns. Emission to water (OECD ESD No. 11, 2004/D 11, p.21).

EE module IC 14A.6: Emission scenario for release of coatings by spray-application from clean-up of mixing apparatus and guns using water back booths. Emission to water (OECD ESD No. 11, 2004/D 11, p.21).

[56] OECD 2004/D11: OECD Revised draft emission scenario document on coating application via spray-painting in the automotive refinishing industry. OECD, Environment Directorate, August 2004.

[57] T_E_16: IC-16 Emission scenario document "Others: Rubber industry", TGD 2003, chapter 7, part IV**.**

Annex 2: The Target Funnel
Results of part A of the OECD Matrix Project

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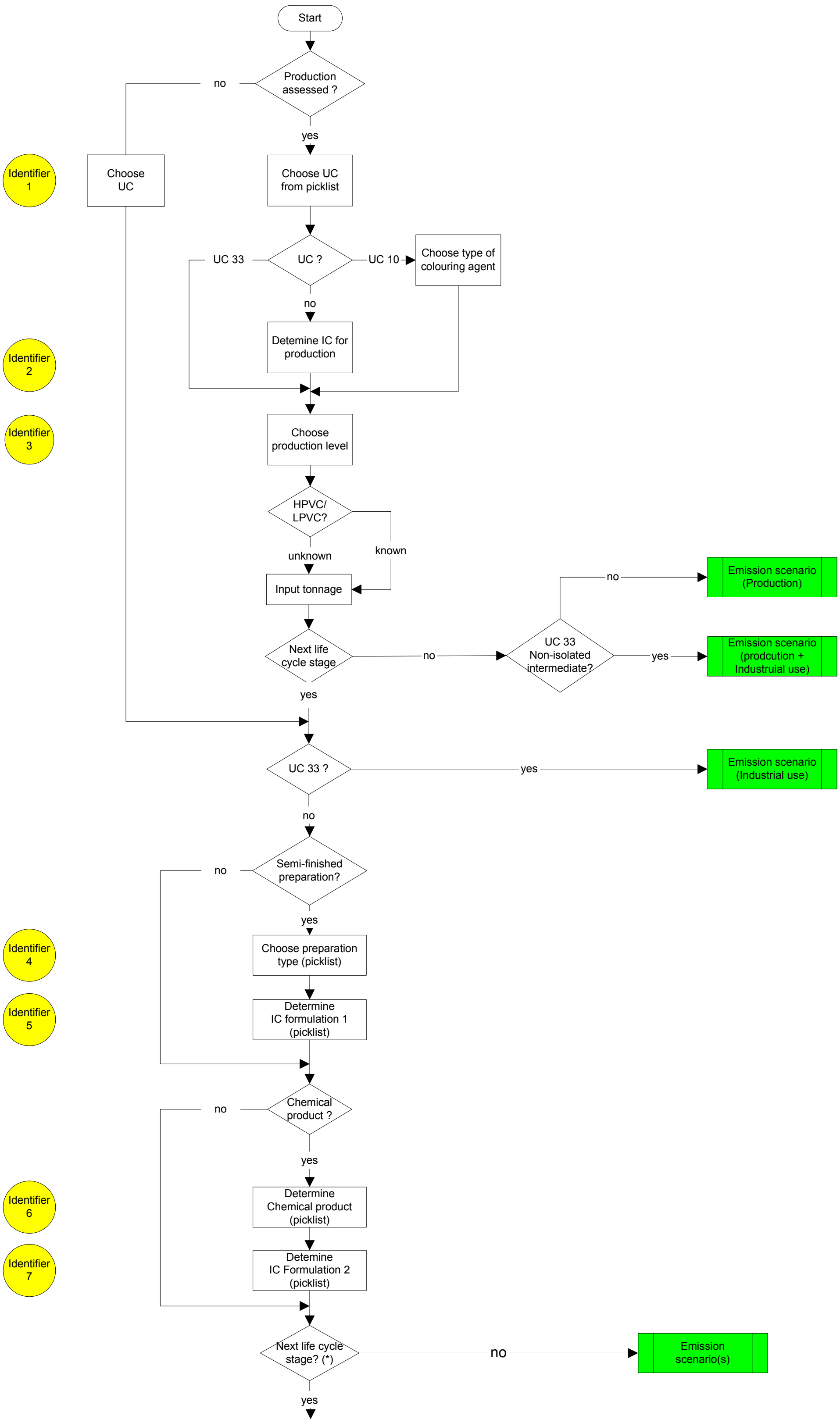
Target funnel for identifying an appropriate emission scenario.

The developed guiding tool, the *target funnel*, implies following (top down) the structure of the decision tree as depicted in Fig. 1 A and Fig 1 B.
The routing through the decision tree is made by the selection of the appropriate values of the so called identifiers.

At this stage, 11 identifiers are applied and named as:

1 Use category
2 Industrial category
3 Production level
4 Semi-finished preparation
5 Industrial category (formulation 1)
6 Chemical products
7 Industrial category (formulation2)
8 Type of use
9 Industrial category
10 Process
11 Any relevant identifier needed

The selection of the appropriate value of the identifier is supported by constructed picklists. The constructed and applied picklists are shown in Figs 2-7, where Figs 2, 3 and 4 are focused on the selection of a coloring agent.



Continued in Fig 6b

Figure 1A First part of the general outline of the decision tree for selection of emission scenarios for the relevant life cycle stages of a substance; (*) if no other life cycle stage have to be assessed the emission scenarios are presented.

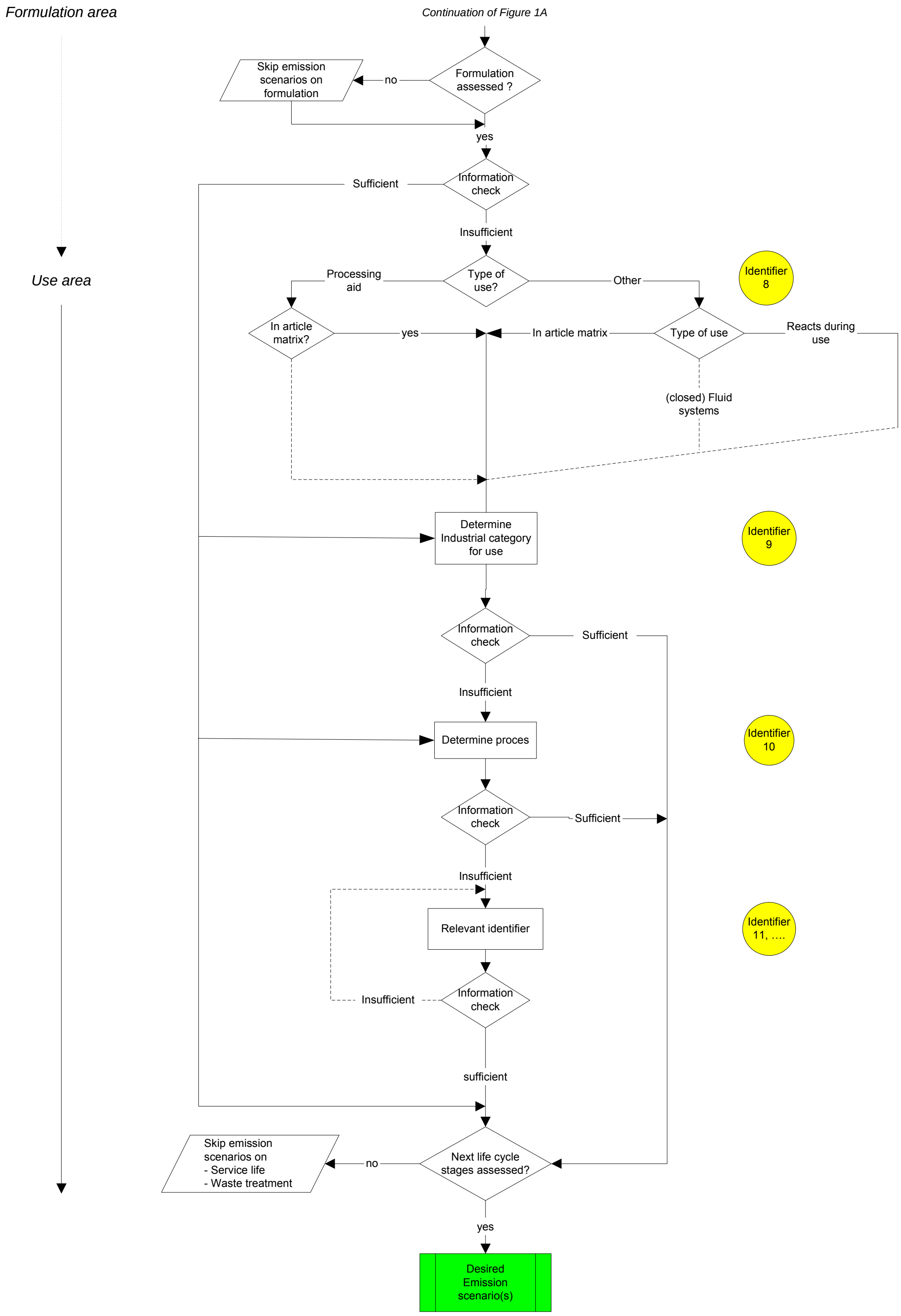


Figure 1B Second part of the general outline of the decision tree for selection of emission scenarios for the relevant life cycle stages of a substance.

Label	Picklist Identifier 1: Use category
UC6	Anti-set-off and anti-adhesive agents
UC9	Cleaning/washing agents
UC10	Colouring agents ⟵ Choice (example)
UC15	Cosmetics
UC20	Fillers
UC27	Fuels
UC29	Heat transferring agents
UC31	Impregnation agents
UC33	Intermediates
UC35	Lubricants and additives
UC38	Plant protection products, agricultural
UC41	Pharmaceuticals (veterinary medicines)
UC43	Process regulators
UC45	Reprographic agents
UC47	Softeners
UC15/0	OTHERS

Figure 2

Picklist for the selection of use categories of the TGD for the stage of production (choice UC 10)

Figure 3

Picklist for the type colouring agent of (choice textile dyes)

Label	Picklist for UC 10 (Identifier 1)
CA1	Leather dyes
CA2	Paper dyes
CA3	Textile dyes ⟵ Choice (example)
CA4	*Combination of CA1 - CA3*
CA5	Other dyes
CA6	Pigments
CA7	Others/Unknown

Label	Picklist Identifier 2: Industrial category (production)
IC1	Agricultural industry
IC2	Chemical industry: basic chemicals
IC3	Chemical industry: chemicals used in synthesis
IC4	Electrical/electronic industry
IC5	Personal/domestic
IC6	Public domain
IC7	Leather processing industry
IC8	Metal extraction, refining and processing industry
IC9	Mineral oil and fuel industry
IC10	Photographic industry
IC11	Polymers industry
IC12	Pulp, paper and board industry
IC13	**Textile processing industry** ⟵ Highlighted (example)
IC14	Paints, lacquers and varnishes industry
IC16	Engineering industries: civil and mechanical
IC15/0	Others

Figure 4

Picklist for the industrial category of the life cycle stage production (IC 13 highlighted because of choice for textile dyes in previous step).

Label	Identifier 4: Semi-finished preparation [1)]
SP1	Dye preparations
SP2	Dyeing auxiliaries (for textile processing)
SP3	Finishing materials (for textile processing)
SP4	Fragrance composition (perfume composition)
SP5	Fuel additives packages
SP6	Lubricant additive packages
SP7	Paint additive packages
SP8	Pigment paste
SP9	Pretreatment agents (for textile processing)
SP10	Surfactant packages

[1)] *Synonyms: Additive pacakage, Performance package*

Figure 5
Picklist for the choice of semi-finished preparations.

	Identifier 6: Chemical product
B1	Antifreezes
B2	Adhesives, blues, sealants
B3	Biocidal products
B4	Car maintenance products
B5	Cleaning products, detergents, soaps
B6	Cleaning products, solvent-based
B7	Coating products (paints, lacquers, varnishes)
B8	Cosmetic products
B9	Fuels
B10	Galvanic preparations
B11	Heat transferring preparations
B12	Hydraulic fluid
B13	Leather dyes
B14	Leather care products
B15	Leather finishing products
B16	Lubricants and greases
B17	Metalworking fluids
B18	Paper chemicals
B19	Paper dyes
	Photochemicals, photographic materials
B20	- for photographic baths
B21	- photographic materials (e.g. films)
B22	Plastic compounds (masterbatches)
	Polishes
B23	- metal polishes
B24	- floor polishes and waxes
B25	- wood polishes and waxes
B26	Semiconductors
B27	Textile dyes
B28	Textile care products (≠ B5 & B6)
B29	Textile coatings
B30	Textile finishing products
B31	Toners

Figure 6
Picklist for the choice of chemical products

Picklist Identifier 8: Type of use		Label
Processing aid	Not in article matrix	TU1
	In article matrix (unintended)	TU2
Other	In article matrix	TU3
	Reacts during use	TU4
	Fluid systems (closed)	TU5

Figure 7
Picklist for the type of use

Annex 3: Overview determinants, data sources and iteration levels in the $EET_{plastic}$ and in the $EET_{photo\text{-}chemicals}$ regarding emission estimation to water

Results of part B2 of the OECD Matrix Project

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Annex 3a

Overview Determinants, data sources and iteration levels in the $EET_{plastic\ additives}$ regarding emission estimation to water for industrial processing

Explanation of symbols

Choices on pick-list	Free text	Defaults	Not implemented in current version of

Abbreviations
M/I = Manufacturer or importer of the substance
F = Formulator of plastic compounds containing the substance
IU = Industrial user converting the plastic compounds into an article
STP = Sewage treatment plant

	Starting point (level 1)	Iteration level 2	Iteration level 3
	Substance properties		
Region	Total market volume		
Back-ground	0.002 regional background emission[1] at 365 days; 80% to STP		
	Dilution 25,000 million m^3/a		
M/I	Own market volume (local)	Own market volume (local)	
		…. Release days/a	
		0.3% emission from process [A 1.1][2]	….% emission from process
		Fraction through STP + dilution volume	
			Fraction to onsite abatement
			Efficiency onsite abatement
F	100% (local)	Fraction main source and release days [B 2.3, B 2.8, B 2.9]	F specific volume[3]
	20 days [B 2.8 (5 t/a)][4]		F specific release days
	0.675 % [highest emission factor from ESD][5]	Emission factors by additive type and process pick-list [ESD]	F specific emission factor (e.g. integrated measures)
	0% through STP treatment, dilution 20,000 m^3/d	Fraction through STP + dilution volume	
			Fraction to onsite abatement
			Efficiency of onsite abatement

[1] 10% of market amount multiplied with medium conservative emission factor averaged across all life-cycle stages (0.3% from M/I; 0.225% from F, processing of > 40 µm particles only; 0.25 from IU due to good process control practice in plastic conversion; 0.84% from service life under the assumption of 25% outdoor use; 0.6% from local waste treatment based on the assumption that only 15% would end up in non-standard landfills; 80% STP connection assumed for all life-cycle stages. The $EET_{plastic}$ does not yet support iteration of these assumptions.

[2] Not clear whether this includes i) integrated measures and/or ii) onsite abatement;

[3] The F, IU and article specific volumes have always to be inserted as a share of M/I's total volume.

[4] Remark: It is recognized that the assumption on the fraction of main source (100% as default = producer sells his total production to one customer) and the worst case assumption on release days from the TGD B-tables is overly conservative;

[5] Raw material handling and compounding for particles < 40 µm and high volatility group (e.g. flame retardant, pigments, antioxidants)

	Starting point (level 1)	Iteration level 2	Iteration level 3
IU	100% (local)	Fraction main source	IU specific volume
	10 days [B 3.9 (10 t/a)][6]	and release days [B 3.9]	IU specific release days
	2.5% [highest emission factor from ESD][7]	Emission factors by additive type pick-list [ESD]	IU specific emission factors (e.g. integrated measures)
		Process temperature driving the emission factor [ESD]	
	0% through STP treatment, dilution 20,000 m^3/d	Fraction through STP + dilution volume Defaults	
			Fraction to onsite abatement
			Efficiency of onsite abatement
Service Life	100% x [1.0][0.1][8]		F/IU or product-type specific volume
Region	365 days	365 days	365 days
	3.2% [organic, outdoor use, 20a service life][9]	Emission factors by additive type + indoor/outdoor use pick-list	Product-type specific annual emission factors + product specific service life
	0% through STP treatment; dilution 25,000 million m^3/a	0% through STP treatment; dilution 25,000 million m^3/a[10]	0% through STP treatment; dilution 25,000 million m^3/a
		Remark: The emission from indoor use to water (80% STP connection as default) can be manually reduced to 30 [50] [70] %, depending on log P and degradability of the additive	Remark: The emission from indoor use to water (80% STP connection as default) can be manually reduced to 30 [50] [70] %, depending on log P and degradability of the additive
Service life	100% x [1.0] [0.002][11]		I/F specific or product-type specific volume
Local	365 days	365 days	365 days
	3.2% [organic, outdoor use, 20a service life][12]	Pick-list additive types + indoor/outdoor use	Product-type specific annual emission factors + product specific service life
	0% through STP treatment; dilution 20,000 m^3/d	Fraction through STP treatment + dilution volume	
Waste	100% x [1.0] [0.1][13]	100% x 0.1	F/IU specific or product-type specific volume

6

7 Grinding/machining of solid additives;

8 A common EU market is assumed from M/I's perspective since usually there is no regional market for plastic additives where M/I would sell his total production volume. Hence the 10% rule applies. However, if the calculation is performed from F's or IU's perspective 100% of volume are assumed since the compounder or converter may have a regional market and hence no "dilution" across the whole market would occur.

9 The emission factor for slip-promoters/lubricants and antistatic agents as suggested in the ESD (100% in 200 days) has not been taken into account for the worst case.

10 The $EET_{plastic}$ does not support yet flexible STP connection depending on the type of article use. However a guided calculation can be carried out manually.

11 It is assumed that the maximum fraction of the registrant's production volume contained in articles in a municipal waste facility can be determined by the fraction of main source for domestic use of chemicals (B-tables) . However, if the calculation is carried out from F's or IU's perspective 100% is assumed by default since the compounder or the converter may possibly serve regional market.

12 The emission factor for slip-promoters/lubricants and antistatic agents as suggested in the ESD (100% in 200 days) has not been taken into account for the worst case.

13 A common EU market is assumed from M/Is perspective since usually there is no regional market for plastic additives where M/I would sell his total production volume. Hence the 10% rule applies. However, if the calculation is performed from F's or IU's perspective 100% of volume are assumed since the compounder or converter may have a regional market and hence no "dilution" across the whole market would occur.

	Starting point (level 1)	Iteration level 2	Iteration level 3
Region	**365 days**	**365 days**	**365 days**
	12.2% (12 + 0.2 metals)[14]	**Pick-list: disposal operation types (emission rates after onsite abatement)**	**Product-disposal specific emission factors**
	0% through STP treatment; dilution 25,000 million m^3/a	**Fraction through STP treatment + dilution 25,000 million m^3/a**	
Waste	**100% x [1.0] [0.002][15]**		**F/IU specific or product-type specific volume**
Local	**365 days**	**365 days**	**365 days**
	4.8% [organic, 30 years open to environment]	**Product-disposal specific emission factors**	**Product-disposal specific emission factors**
	0% through STP, 20,000 m3/d	**Fraction through STP treatment + dilution volume**	

[14] Highest emission factor for waste remaining in the environment from the EU RAR on DEHP assessment (coil coated roofing sheets: 50% of which 25% goes to water).

[15] It is assumed that the maximum fraction of the registrant's production volume contained in articles in a municipal waste facility can be determined by the fraction of main source for domestic use of chemicals (B-tables). However, if the calculation is carried out from F's or IU's perspective 100% is assumed by default since the compounder or the converter may possibly serve regional market.

Annex 3b

Overview Determinants, data sources and iteration levels in the EET$_{photochem}$ regarding emission estimation to water for industrial processing

	Starting point (level 1)	Iteration level 2	Iteration level 3
	Substance properties		
Region Back-ground	Total market volume		
	[2.21%] regional background emission[16] at 365 days; 80% to STP;		
	Dilution 25,000 million m^3/a		
MI			
F			
IU	Own handled volume (local)	Area of processed material pick-list and concentration in bath pick-list [ESD] (leading to own handled volume)[17]	Area of processed material
			Bath concentration
	300 emission days [B 3.8][18]		
		Bath-type, concentration in bath, ingredient-type and CO or RP rate by pick-list (leading to emission factor) [ESD]	CO rate RP rate
	100% emission [ESD[19]]	Substance specific removal due to reaction on use (leading to emission factor) [ESD]	Substance specific removal
			Fraction to onsite abatement
			Efficiency of onsite abatement
	0% through STP treatment, dilution 20,000 m^3/d	Fraction through STP + dilution volume	Fraction through STP + dilution volume Fraction Onsite abatement
Service Life Region			

[16] Calculation as in the case of plastic additives (see footnote 1 of annex 3a). Not valid for photo-chemicals
[17] This is the ESD-route to determine the substance volume (= "fraction of main source") and ideally it should match with volume inserted in the beginning of the first iteration. Could be brought into the TGD B table format (just by manual conversion) in the follow-up-project
[18] Default value from the TGD table B 3.8.
[19] This is the default value for process baths with direct discharge to wastewater and no removal of the substance during the process (according to the ESD)

	Starting point (level 1)	Iteration level 2	Iteration level 3
Service Life			
Local			
Waste			
Region			
Waste			
Local			

Explanation of symbols

Choices on pick-list

Free text

Defaults

Not implemented in current version of the IT tool

Abbreviations
M/I = Manufacturer or importer of the substance
F = Formulator of plastic compounds containing the substance
IU = Industrial user converting the plastic compounds into an article
STP = Sewage treatment plant

Annex 4: Flyer and presentation of the IT-Tool

Results of part B2 of the OECD Matrix Project

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ENVIRONMENTAL EXPOSURE ASSESSMENT UNDER REACH

Piloting branch- and product-related emission estimation tools for manufacturers, importers, and downstream users

Tool for Additives used in Plastic Compounds (Pilot)

The REACH Requirement

Under the REACH regulation, manufacturers and importers of dangerous substances (above 10 t/a) have to describe the conditions of safe use and to communicate these to their customers. For that purpose the manufacturer has to define suitable exposure scenarios and to carry out an exposure assessment for the whole life cycle of his substances. The direct customer and his subsequent customers each have to implement the conditions and measures communicated to them, or to adjust the scenario under their own responsibility, respectively.

The Challenge

Implementation of these requirements may be a difficult task for industry, due to a number of reasons:

- Manufacturers often do not know much about the uses and the conditions of use in their markets, in particular regarding uses beyond their direct customers. Also, the information available from EU and OECD Documents is not recognised and used by manufacturers yet.
- Many downstream users are used to comply to emission limit values (if existing) but lack expertise and skills to carry out systematic exposure assessment and risk characterisation for all substances they handle.
- All actors in the supply chain do not yet have a common language and standard procedures to communicate on product safety up and down the chain.

The Approach

The German Federal Environmental Agency (UBA) has initiated two R&D projects aiming at the development of easy to use, IT supported tools. The tools are designed in a way that suppliers and users can contribute information on the conditions of use consecutively into a common framework. The branch-specific tools are developed in close co-operation with the respective industry sectors: textile finishing, plastic additives, and photochemicals. The tools can be easily adjusted to the needs of other sectors since they are based on a set of generic formulas and a set of generic determinants for emissions:

- Amount of substance handled per day or year at a site or contained in an article
- Emission factor driven by the technical conditions of use (characterised by a number of life-cycle-stage or branch specific determinants)
- Emission reduction by on-site abatement or product integrated safety measures
- Emission reduction by external risk management measures, like municipal waste water treatment

The tools are designed for emission estimates, but they both include exposure assessment and risk characterisation for the water compartment. This is to illustrate the whole CSA process in the tool. The tools translate the OECD Emission Scenario Document (ESD) and the TGD emission calculation rules into a guided, stepwise emission estimation process and corresponding pick-lists with emission factors. The application of risk management measures has been additionally integrated into the tool.

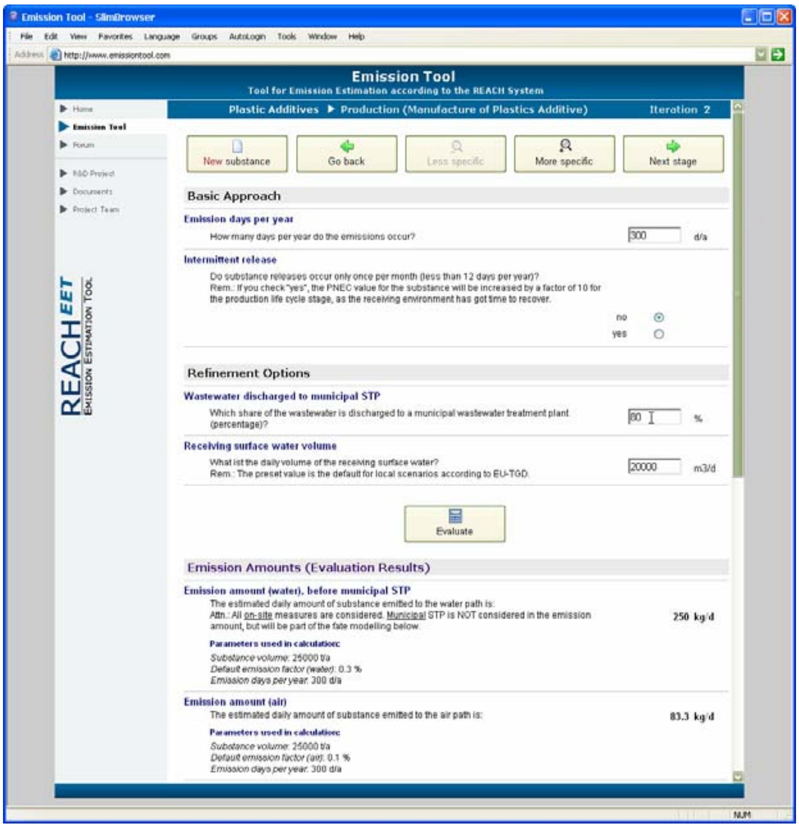
Emission Estimation Tool (EET) for Plastic Additives

The EET for additives in plastic is a flexible Java based web application using XML techniques to store all control data. Thus the tool could easily be adapted to other supply chains by adding their control data as XML documents. The tool can be found at http://www.emissiontool.com. It is open to the public and everyone is invited to try it out. The tool is not yet suitable to carry out a *full* exposure assessment under REACH though.

At each of the five life cycle stages, three levels of preciseness exist (iteration level 1-3). From level 1 to level 3, conservative defaults can be replaced consecutively with more specific information if needed.

In order to integrate a driver for iteration, at each life cycle stage and iteration level a PEC/PNEC ratio for the water compartment can be derived. If it is < 1, the assessment is finished. Fate and exposure is calculated based on the TGD rules for a local scenario and a regional scenario. Although not required by REACH, a regional background PEC is calculated in order to inform the individual company whether a risk at EU level may exist due to multiple emission.

The assessment process can also be carried out by the compounder or the converter, given the relevant substance information has been inserted. Once a user has identified himself as a compounder or converter the program adjusts itself to this user. Since the web application does not yet support interim storage of data, level 1 or 2 iteration cannot be handed over from the manufacturer to his customer. However, this is simply a matter of further development.



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