R+D Project FKZ 204 67 456/02

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

OECD Matrix Project

IT Design Document

for the Emission Estimation Tool (EET)

Part II of supplement M 5

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1. Introduction

1.1. Purpose

This document is the design document for the [EmE tool] [1] to be developed within project phase B2 of the [ESD matrix project]. The purpose of this document is to provide the design for a software application to carry out standard emission calculations.

It is based on the [Outline design doc] delivered 20-Apr-2005 and has been extended by an analysis of the required dialog steps and the input and output values involved. The results of this analysis are summarized in the "user dialog sequence" (⇨annex I). It has also been revised to include the conceptual developments that have taken place in the meantime.

- Chapter 1 explains the purpose of this document (1.1), the scope of the current project (1.2), and the methods applied for creating of this document (1.3).
- Chapter 2 provides references to other documents created within (2.1) or outside (2.2) the current project.
- Chapter 3 lists document specific abbreviations (3.1) and terms (3.2).
- Chapter 4 gives an overview of the main objectives of project phase B2.
- Chapter 5 explains the technical guidelines developed within project phase B2 by the [project team].
- Chapter 6 describes IT requirements to be observed.
- Chapter 7 gives a brief overview of the proposed IT system.
- Chapter 8 outlines the architecture of this system. Functional and data modelling aspects are discussed in 8.1, followed by a conceptual design of the user interface (8.2).

- Annex I contains the conceptual analysis of the user dialog sequence. It has been developed on the basis of the [IT guidance plastic additives] prepared by Oekopol Institute within the current project.

The *design document* maintains and updates the [Outline design doc]. Chapters 1 to 6 have been revised, chapter 7 now covers the IT system in greater detail, and chapter 8 has been thoroughly revised to comply with the user dialog sequence developed in the meantime.

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1 Each first occurrence of a term or abbreviation is surrounded by square brackets. All such terms and abbreviations are explained in chapter 3.

1.2. Scope

According to [Offer 12-Aug-2004], the project scope is defined as follows:

> *"… to develop a set of technical guidance documents (manual and software-tools) for emission and subsequent exposure estimation as outlined in annex 1 of the draft REACH Regulation. Such guidance shall be robust and easy to use by manufacturers, importers and downstream users of substances. The conceptual approach shall be based on the methodology laid down in EU TGD on Risk Assessment of New and Existing Substances and the OECD Emission Scenario Documents (ESD). In addition the tool is expected to fit into the EUSES methodology. …"*

In the meantime, it has been clarified that the current project has its focus on all aspects of *substance emission*, rather than *fate modelling* and subsequent *calculation of environmental concentrations* [PEC]. For various branches of industry, OECD [ESD]s have been published that analyze the specific industrial and professional processes with respect to substance emission. Emission calculations based on ESDs are thus branch- and – in most cases – also product- / process-specific. They can still be considered to be *standard* emission calculations, as ESDs do *not* refer to the individual situation of specific actors in the supply chain.

In cases where no information from ESDs is available, standard emission scenarios from the relevant EU [TGD] will have to be used instead. Emission calculations according to TGD are based on values taken from [A/B tables].

Therefore, the scope of the EmE tool to be developed covers *standard emission calculations* based on ESDs and TGD.

To demonstrate its usefulness to the *exposure scenarios* according to REACH, the EmE tool will be extended by a *fate module* allowing for the calculation of PEC values, including mechanisms for a PEC / PNEC comparison and subsequent iteration cycles, if needed.

1.3. Methods Applied

The development of the EmE tool is part of project phase B2, comprising *"manuals and software tools"* according to [Offer 12-Aug-2004]. The manuals have been created for the supply chain "plastics additives" by the [consortium] members Öko-Institut and Ökopol Institute, thus defining an interface for the IT development carried out by the third member of the consortium, Chemie Daten.

Interface between manuals and IT development

For the exemplary supply chain "plastic additives" the [Manual plastic additives] comprising the scientific background and the necessary parameters and calculation models has been prepared within the current project.

It is supplemented by an [IT guidance plastic additives] which concentrates on the necessary information for IT development, i.e. parameters and calculation algorithms, and contains further specifications. It is intended as an "interface" between [Manual plastic additives] and IT development.

The [IT guidance plastic additives] has in turn been extracted for the preparation of the user dialog sequence (⇨ annex 1). This document includes all the dialog steps with the respective input/output values and display texts that are relevant for the supply chain 'plastics additives'.

The [Manual plastic additives] was developed jointly by Öko-Institut and Ökopol, the [IT guidance plastic additives] by Ökopol. The user dialog sequence (⇨ annex I) was prepared by Chemie Daten on the basis of the [IT guidance plastic additives].

The [Manual plastic additives] was presented to and discussed with representatives from the plastics additives industry on a workshop which has taken place on 07-Jul-2005 in Frankfurt.

The feedback from this workshop has been included in the [Manual plastic additives] and subsequently transferred into the [IT guidance plastic additives].

However, the [Manual plastic additives] is the reference document for all scientific issues.

Preparation of the IT outline design document

A first internal meeting of the project group took place on 14-Feb-2005. The outcome of this meeting, together with a series of subsequent telephone conferences, provides the material for the generation of an <u>outline</u> design document for the software tool to be developed.

The outline design document has been delivered by 20-Apr-2005.

Preparation of the IT design document

A design document was originally planned to be prepared in June 2005. Since this document is intended for internal use only, the project partners have come to the conclusion that it would be preferable to reduce the original scope of this document in favour of extra resources gained for software development.

Development, testing and deployment of the EmE tool

According to current planning, a first prototype of the EmE tool will be presented by October, 2005. It will cover the supply chain "plastics additives".

An extensive testing phase is then scheduled for the months of October, November and December. All project partners should be involved in this testing period, as well as selected stakeholders from both supply chains.

By the end of the year, the prototype version of the EmE tool should have been expanded and consolidated to an extent that it can be granted the status of a "project deliverable".

Further enhancement, refinement and debugging that might be necessary on a limited scale could then be carried out within warranty responsibilities.

2. References

2.1. Applicable Documents

Documents created as a deliverable in the current project are quoted by specific abbreviations, surrounded by square brackets, e.g. "… [Offer 12-Aug-2004] …".

Following is the list of applicable documents:

quotation	document reference
Final Report A	"Final Report for Project A. Technical guidance for identifying the appropriate emission scenarios", National Institute for Public Health and the Environment (RIVM), 02-Aug-2005
IT guidance plastic additives	"Documentation of IT-logics for developers" for the 'plastic additives' supply chain. Prepared by A. Reihlen, Ökopol, 30-Aug-2005
Manual plastic additives	"Manual for emission estimation of plastic additives". Jointly prepared by Öko-Institut and Ökopol, 01-Aug-2005
Offer 12-Aug-2004	Offer by Öko-Institut, Ökopol Institute and Chemie Daten, based on the tender issued by Umweltbundesamt on 29-Apr-2004. The contract defining the current project is based on this offer.
Outline design doc	"Design Document for a Software Application Supporting Branch and Product Related Emission Estimation (EmE Tool) v 1.0" by Chemie Daten, 20-Apr-2005
Tender 29-Apr-2004	"Tender (Sub-Project B) - Branch- and product-related emission estimation tool for manufacturers, importers, and downstream users within the REACH-system", Umweltbundesamt, 29-Apr-2004

2.2. Reference Documents

Other documents are also referenced by abbreviations in square brackets. Following is the list of referenced documents, except for the applicable documents:

[none]

3. Abbreviations, Terms and Definitions

3.1. Abbreviations

In this document, the first occurrence of an abbreviation is marked by square brackets.

Following is the list of abbreviations and their respective explanations:

abbreviation	explanation
CSR	Chemical Safety Report
ESD	General abbreviation for OECD "Emission Scenario Document". A total of 17 ESDs have been published ("declassified") by OECD or are currently under discussion.
IC	industrial category according to TGD
MC	main category according to TGD
PEC	Predicted Environmental Concentration
PNEC	Predicted no effect concentration (usually referring to aquatic media)
RMM	Risk Management Measures according to TGD
STP	Sewage Treatment Plant
STM	Simple Treat Modelling. Calculation model for sewage treatment in accordance with TGD.
TGD	General abbreviation for EU Technical Guidance Document, in this document TGD always refers to the "Technical Guidance Document on Risk Assessment – Part II"
UC	use category according to TGD

3.2. Terms and Definitions

In this document, the first occurrence of a specific term or definition is marked by square brackets.

Following is the list of terms and definitions, together with an explanation in the context of this document:

term or definition	explanation
A/B tables	A- and B-tables are published as an annex to TGD (see 3.1). These look-up tables provide various specific values needed for standard emission calculations according to TGD.
consortium	The current project is carried out by a consortium of three institutes: Öko-Institut (Freiburg), Ökopol Institute (Hamburg), and Chemie Daten (Berlin).
EmE inventory	Database, in which all specific data for the individual emission scenarios are stored: emission relevant factors, input parameters, calculation and look-up rules, dialog control etc.
EmE module	Emission estimation module – base element of the EmE tool, each EmE module being assigned to a specific life-cycle stage and environmental compartment. Setting up the EmE tool from EmE modules as "building blocks" provides for a modular functional software design.
EmE tool	Software application to be developed within the current project.
ESD matrix project	Current project – full title: *"Branch- and product-related emission estimation tool for manufacturers, importers and downstream users within the REACH-system"*, R+D Project FKZ 204 67 456/02, 09/2004 – 11/2005, by German Umweltbundesamt.
EUSES	The "European Union System for the Evaluation of Substances" is a PC program designed as a decision-support system for the evaluation of the risks of substances to man and the environment. It is based on EU TGD for the risk assessment of new and existing substances and biocides.
fate module	Fate estimation module – element of the EmE tool, that can optionally be carried out after an emission estimation. If selected, the daily emission rate will be fed into the fate module to calculate an environmental concentration (PEC) for the water path.
project team	All three members of the consortium contribute to the project team. Currently, the project team consists of: Dr. Dirk Bunke (Öko-Institut), Mr. Andreas Ahrens and Ms. Antonia Reihlen (Ökopol), Mr. Hans-Peter Schenck and Mr. Marcus Oenicke (Chemie Daten).

4. Objectives

This chapter describes the objectives, as they are specified in the contract for project phase B2 in the ESD matrix project.

4.1. Branch and Product Related Approach

While the EU TGD follows a more generic approach, the design of the EmE tool will be able to accommodate branch-specific parameters. This is also the approach of the OECD ESDs. It is expected that this will produce better results and increase acceptance by the stakeholders of the supply chains. It is in this sense that the EmE tool will follow a "branch-related" approach.

The EmE tool will also be "product-related" in a sense that it follows a specific substance through the various "products" in which it occurs during its life-cycle. A bulk chemical produced by an industrial producer is a "product" in this sense. It is supplied to a formulator producing preparations, which in turn are *his* "products". There may be secondary formulators who combine "performance packages" of primary formulators into preparations as their "products". These are eventually passed on to industrial, professional or private users.

4.2. Use of OECD ESD and EU A/B Tables for Emission Calculation

According to [Tender 29-Apr-2004] both OECD ESDs and TGD (A/B) tables are to be used as the basis for standard emission calculation.

The calculation model will be compatible with the TGD approach, but it is <u>not</u> the aim of the EmE tool to rival the complex logic of the [EUSES] application. Instead of covering the risks of a substance for man and environment on a local, regional and even global scale, the EmE tool concentrates on delivering emission estimations for individual life-cycle stages and environmental compartments. The individual results can then be used for further calculations or fate models.

For this purpose the aggregated values of the A/B tables are quite sufficient. ESDs offer calculation models for specific branches and product groups that need to be analyzed and employed for the EmE tool. Since the ESDs follow no common structure the extraction of calculation models for the individual life-cycle stages of each analyzed supply chain is the key task of project phase B2. This (non-IT) task has been carried out by the consortium members Öko-Institut and Ökopol and is integral part of the work for the manual but is not part of the IT development.

4.3. Emission Drivers

From a conceptual point of view, the relevant *emission drivers* are as follows:

- *amount of substance [per year]*
- *number of release days [per year]*
- *release scale [local / regional]*
- *loss from production / use [percentage]*
- *emission reduction by on-site abatement [percentage]*

In order to carry out emission estimations for the different life-cycle stages within a supply chain, the checked emission drivers need to be considered individually.

	P Production	**F** Formulation	**IU** Industrial Use	**PU** Professional Use	**CU** Consumer Use	**SL** Service Life	**W** Waste[2]
amount per year	✓	✓	✓	✓	✓	✓	✓
release days	✓	✓	✓	✓	✓	✓	✓
release scale	✓	✓	✓	✓	✓	✓	✓
loss from production	✓	✓	✓	✓	✓	✓	✓
on-site abatement	✓	✓	✓	✓	✓	✓	✓

To carry out emission estimations, various individual *parameters* relevant for the emission have to be entered and processed. The evaluation of all these parameters leads to an *emission factor*, describing the fraction of a substance emitted at the life-cycle stage under consideration. From this, the daily *emission rate* is calculated in combination with other parameters (e.g. amount per year and release days).

Emission factors and their underlying parameters will usually have different values in different life-cycle stages. If calculations are necessary to determine a factor, these can also vary between life-cycle stages.

Thus, specific parameters and calculation algorithms (formulas) have to be considered for emission estimation within each life-cycle stage.

2 "Waste" in this context stands for: "Waste / Waste water treatment/management"

4.4. Emission Calculations along the Substance Life-cycle

For each life-cycle stage of a substance under consideration, i.e. every column of the life-cycle shown in chapter 4.3, the EmE tool will offer emission estimations. These estimations will have to take into account all environmental compartments, as follows:

- *air*
- *water*
- *soil*

This leads to a maximum of three formulas (emission modules) per life-cycle stage.

Waste will not be implemented as a separate emission path within the scope of this project. Calculations for this emission path are, in fact, difficult. Often indirect measures are applied to obtain emission estimations for the waste compartment. However, waste is covered as a final *life cycle stage*.

Each of these individually defined emission modules may need to be applied repeatedly with a different number of parameters to fully cover the emissions along a life-cyle. This will be particularly true for the life-cycle stages *formulation* and *service life*, where more than one scenario might have to be carried out in parallel.

4.5. Extension to Fate Modelling

The current project has its focus on *substance emission*, rather than fate modelling and subsequent calculation of environmental concentrations (⇨ chapter 1.2). The drawback of this approach is that the emission estimations carried out by the EmE tool will not be sufficient on their own for conclusions within REACH.

Without a [PEC] no comparison of PEC / [PNEC] is possible and without this the stakeholders of a supply chain will not be able to decide upon the need for action according to REACH.

To overcome this disadvantage, the EmE tool will be extended by an extra module with an exemplary fate model for the emission path "water", which will allow for an estimation of:

- *PEC in surface water (local / regional)*

If PNEC values for this environmental compartment are available to the user, PEC and PNEC can be compared. If this leads to the need for action according to REACH, the EmE tool will offer an iteration cycle. This aims at a more precise estimation and a better reliability of the resulting PEC/PNEC ratio.

5. Approach

The objectives according to chapter 4 summarize the key aspects of the [Manual plastic additives]. These are further specified in the [IT guidance plastic additives], which has the function of an interface between the [Manual plastic additives] and IT development. This interface consists of precise conceptual guidelines for building the EmE tool.

Chapter 5 focuses on the essentials of the guidelines described in the [IT guidance plastic additives] and reflects the logical structure of the user dialog sequence (⇨ annex I).

5.1. Product Supply Chains

While the EmE tool should be expandable to any industry branch / supply chain, it will be implemented for all relevant life-cycle stages and environmental compartments of a model supply chain. For this, "plastics additives" have been chosen.

It is planned to illustrate the adaptability of the EmE tool to other supply chains by implementing selected EmE modules from the supply chain "photo chemicals" that are especially suitable for demonstration purposes.

5.2. Substance Functions

Emission estimations for substances depend to a great extent on the product type they are applied on. Therefore, the *substance function* needs to be taken into account, as emission estimations always refer to the substance level.

As a result of project phase A ("funnel project"), a procedure has been developed to identify the applicable ESD guidelines with the help of the categorization schemes [IC] and [UC]. The practicability of the NACE codes was also investigated, but it turned out that the NACE has little relevance as yet. The concept of the "target funnel" is explained in detail in [Final Report A].

5.3. Life-cycle Stages

Emission estimations should generally be possible for all stages of the substance life-cycle under consideration. As not all of the life-cycle stages are relevant in any case, a selection will be necessary under the *potentially* relevant life-cycle stages, as follows:

- production
- formulation
- industrial use
- professional use
- consumer use
- service life
- waste

5.4. Standard Emission Estimation

A key aspect of the EmE tool will be its flexibility, allowing for extension to other supply chains as needed.

In order to achieve this, all standard emission calculations need to conform to a common design and structure.

For each combination of a life cycle stage and an environmental compartment specific *emission parameters* as well as *calculation and look-up rules* are stored. Together, these correspond to exactly one *emission estimation module*.

All specific information on parameters and calculation / look-up rules is stored in the EmE tool's repository ([EmE inventory]).

5.4.1 Emission Parameters (Standard Input)

Emission parameters are the parameters needed for estimating the daily emission rate. Three categories of emission parameters are to be distinguished, as follows:

Product and Substance Related Parameters

These parameters are valid for a given product/substance and are applicable to any supply chain or life-cycle stage. The following parameters are relevant for emission estimations, not all of them needed each time, though.

- Molecular weight (MW)
- Vapour pressure (Vp)
- Solubility in water

- Partitioning coefficient octanol/water (log Pow)
- Physical state (e.g. "dustiness")
- Degradability

Process Related Parameters

These parameters are specific for a given supply chain and life-cycle stage. They will be used in all kinds of emission estimations.

- *Amount of product/substance used per year*

  The default value for 'fraction of main source' will be taken from B-tables (no default for life-cycle stage *service life*). It may be overwritten according to the user's own knowledge of the production volume.

- *Release days*

  The default value will be taken from B-tables and may be overwritten according to the user's own knowledge.

- *Release scale*

  The default will be "local", but may be changed to "regional".

- *Loss from production / product*

  This is the fraction of product or substance that is lost from the process / from the product *(service life)* into environmental compartments. The default values will be taken from ESDs or A-tables.

- *On-site abatement (process integrated RMM)*

  Abatement measures may be directly integrated into the production process, e.g. recovery measures. They lead to deductions from the process related factor "loss from production". Abatement factors are always site specific.

Parameters Related to On-Site Abatement

In addition to process-integrated abatement separate "end-of-pipe" measures need to be considered, e.g. on-site waste water / waste gas treatment.

- *On-site abatement (end-of-pipe RMM)*

  These denote measures which can be applied in succession to several production processes and lead to a *collective* deduction in emission.

In general, abatement measures are specific for a given production site. Default values will only be used on a worst case basis.

On-site abatement factors are, within REACH, equivalent to – and due to – risk management measures [RMM]. For each process, a number of RMMs may be applicable, but which of these are actually employed depends on the conditions and policies of the individual production site. Therefore, on-site abatements will *not* be activated for default calculations, but offer the most options for refinement.

5.4.2 ESD vs. A/B Tables: 'Best Available Method'

Since both OECD ESDs and TGD A/B tables are used for emission estimation (⇨ chapter 4.2), two approaches are possible:

1. *"Phased approach"*

   The EmE tools uses the values derived from the A/B tables for a *default calculation*. If available, the ESD model is offered as a *refinement option*.

2. *"Best available method"*

   ESD model calculations are used whenever possible. A/B table values are used only if no ESD model is available.

For the EmE tool, the second approach will be used. It does not seem to make much sense "hiding" the more precise model behind broader default values. Also, A/B tables are not available for all supply chains and life-cycle stages, anyway.

5.4.3 Daily Emission Rate (Standard Output)

Technical processes are often not carried out continuously, but in batches, and therefore production need not be spread evenly across the year. Since the emission estimation is based on the *relevant* periods of time, it is calculated on the basis of production days and <u>not</u> as an average value per year.

The target value of all emission estimations is therefore the amount of substance that is released into the environmental compartment of interest *per day*:

- *daily emission rate to surface water*
- *daily emission rate to ambient air*
- *daily emission rate to soil*

5.5. Exposure Estimation (Water Path)

In addition to the emission estimation the EmE tool will also be able to make an estimation of the exposure to the environment. As this is not covered by the scope of this project, it will be created as an exemplary add-on, covering the water path.

Because of the exemplary nature, the fate modelling required can be kept simple. Instead of complex calculations, it will be based on standardized values derived from the TGD.

The exposure estimations are directed at *predicted environmental concentrations* (PEC) in surface water. It will take into account the local scenario and possibly also a regional scenario.

5.5.1 Fate Parameters (Extended Input)

For fate modelling extra input parameters will be needed apart from the emission parameters listed above (⇨ chapter 5.4.1), as follows:

Product and Substance Related Parameters

For modelling the way through a sewage treatment plant [STP] extra intrinsic substance properties may be needed from the list shown above (⇨ chapter 5.4.1).

Dilution Related Parameters

The receiving water volumes (both waste water and surface water) are parameters used for dilution estimation.

PNEC

The PNEC is a substance related value assessed by ecotoxicological tests. It is known by all stakeholders along the supply chain. The PNEC is needed for PEC/PNEC comparison (see below).

5.5.2 PEC/PNEC Comparison (Extended Output)

The exposure estimation will allow for a PEC/PNEC comparison (water path only). To achieve this, the following standard calculations need to be carried out:

- *STP Modelling*

  For simulating the treatment in an external STP factors derived from the Simple Treat Model according to TGD are applied. The modelling is carried out with defaults from the A/B tables.

- *Dilution Estimation*

  The receiving water volume needs to be estimated for the STP (waste water dilution) as well as the surface water (surface water dilution). For both parameters either exact values can be used, or defaults according to TGD.

  The use of *STP modelling* and *dilution estimation* results in a PEC value, or different values for local and regional scenarios, if applicable.

- *PEC/PNEC Comparison*

  Finally, the EmE tool compares the determined PEC with the known PNEC. If the PEC/PNEC ratio is greater than 1, it indicates that admissible exposure levels are exceeded in the selected emission/exposure scenario.

5.5.3 Refinements / Iteration Cycles

A PEC/PNEC ratio > 1 signals need for action to the stakeholder involved. In this case the estimation should be repeated with more precise values and the resulting PEC/PNEC ratio re-examined for compliance of the exposure level with REACH requirements.

Such iteration cycles will be supported by the EmE tool to demonstrate an application of emission rates.

6. IT Requirements

The EmE tool is intended to be made available to a large number of potential users, but will be used by these as the occasion arises, i.e. intermittently. This leads to a series of basic IT requirements, as follows:

Easy-To-Use Software Design

The software should be simple, intuitively to use and mostly self-explanatory. This assumes that the user has a basic knowledge of the subject involved. "Emission" and "exposure estimation" should be familiar terms to him or her.

Robust Implementation

The software should be running without errors. User entries should not lead to malfunctions or cause the application to crash.

No License Requirements

The use of the software should be licence-free. This applies to all software-components including those that may be needed on the user's computer.

Broad and Direct Accessibility

The EmE tool is intended to be distributed to a broad community of occasional users. Therefore, direct and uncomplicated accessibility to the EmE tool is essential.

Local installations requiring a setup routine are adverse to accessibility, simply because users often lack sufficient (administrator) rights and need the support of an adequately authorized person. Also, in many institutions policies will not allow individual installations of software applications for the occasional use.

Modular, Extensible Design

The matrix design of the project as a whole already suggests a modular design of the software. It is obvious that individual programming of all emission modules (per life-cycle stage and environmental compartment) could <u>not</u> be considered an adequate solution.

Furthermore, the design of the EmE tool is required to allow for more supply chains to be added later on.

This leads to a software architecture organizing functionalities into small, reusable components. These components (or: modules) need to be controlled by a central logical unit that determines the program flow. The logical unit has to be designed in a way that new demands (i.e. extra supply chains) can be integrated later on.

Storage of Input Values and Results

It will be a common situation that the use of the EmE tool needs to be interrupted for a certain time, e.g. to look up specific values for input. This will particularly be the case if refinement options are required and the necessary information are not at hand.

Therefore, a fully completed EmE tool will need to provide mechanisms to save the values already entered as well as emission estimations calculated. The stored information must be easily accessible at a later time, either to finish with an interrupted input situation or to repeat calculation with refined input values.

Interface Support

The EmE tool will allow the stakeholders of a supply chain to carry out emission estimations in a standardized way. The calculation modules are designed in a simple and comprehensible way. Complex calculations will be avoided within the EmE tool.

In those cases where emission or exposure estimations indicate the need for action, more detailed calculations will be required. These will be carried out by other calculation models in external programs, but the EmE tool should pass on existing data.

Therefore, the EmE tool will have to provide *export mechanisms* that allow for the transfer of input parameters as well as calculated values like emission estimations to such programs like EUSES or maybe other TGD compatible software using the *Simple Treat Model*.

Standardized formatting conventions for chemical safety reports [CSR] will *not* be provided within the time frame of this project.

7. System Overview

This chapter describes the major topics of an IT system to implement the requirements depicted in chapter 6.

Software Platform

The platform proposed is a server based application with standardized access mechanisms via internet (web application).

The logic of the application will be completely located on a central application server (web server) and be freely accessible through the internet. The EmE tool will be started from and running in an internet browser (Internet Explorer, Mozilla Firefox, Netscape) on the user's computer.

No local setup routines will be needed for this and also no downloads of files that would need to be installed locally.

This platform has been chosen to meet the requirement of direct availability of the EmE tool to a large number of occasional users.

Modular Design

Central unit of the EmE tool is a single emission module within the life-cycle under consideration. This unit contains all functions needed for an individual emission estimation (initial questions, input of relevant parameters, determination of emission relevant factors, estimation of *daily emission rate* (⇨ chapter 5.4).

This emission estimation module [EmE module] is linked with a data source in which the individual definitions of the different emission scenarios in the EmE tool are stored (emission estimation inventory, [EmE inventory]). The combination of an EmE module and its related records in the EmE inventory represents the functionality required for a single specific emission estimation.

Another basic module of the EmE tool is a standardized *exposure estimation module* [fate module] for the water path that will automatically be carried out as an extra estimation step for calculating a PEC value (⇨ chapter 5.5).

EmE (and optionally fate) modules are invoked by the central control logic in which all general parts of the overall logical sequence are defined.

The control logic is also linked to a data source with parameters (definition of supported supply chains, life-cycle stages etc.), thus making it flexible and adaptable.

This architecture is the basis for extending the EmE tool with more supply chains, substance life-cycles and possibly even extra add-on modules for other fate models at a later time. All extensions will be possible with a comparatively small effort.

User Interface

The program will be started and run solely within a standard internet browser. The user dialogs will therefore have a design that is "typical" for internet applications. They will be clear and straightforward and there will be no need for "fancy" graphics.

Operating the EmE tool should be possible without the need to consult a manual, but all dialog steps will include short explanations of their purpose and will be supplemented by more detailed comments as the situation requires. They can be opened on demand by the user.

Navigation Basics

The program sequence is basically linear. Starting from the main menu, the various selections and input of parameters will be gone through until the emission estimation is calculated. By default, fate modelling is carried out for the water path. On the level of life-cycles stages, more emission estimations for other environmental compartments may be carried out. Eventually, the user can decide to a) select another life-cycle stage for calculation, repeat the calculation for the same life-cycle stage with different input values or c) to go back to the main menu.

The data entered by the user are intended for the current application context only. This context is defined by the supply chain chosen. Data will be maintained within this context, but they will not be stored permanently for later use. Since returning to the main menu is equivalent to leaving the current context defined by the supply chain, previous input data and results will be discarded at this point.

Iteration cycles and refinements are offered wherever the optional exposure estimation module indicates a PEC/PNEC ratio above 1 and, consequently, the need for action. Context and relevant data are maintained for a new estimation cycle using existing input data as default values that may be edited by the user. The same applies to the calculation of further life-cycle stages within the same supply chain.

Software Limitations

The task of storing input values and results of emission estimations for later use is not trivial within a web application.

This is due to the fact that the "intelligence" of the application is located on the (web) server, while the user works with the application's *representation* in the browser. Therefore, all data entered and results produced are located on the server, not on the user's local computer.

A second reason is that users are "anonymous" in standard web applications. This is to say, the server notices only the fact that a new user is starting the application ("session"), but not who he is. While the application is running, the server uses a "session id" to keep track of the user's movements. Once the application is closed by the user (closing the browser window or moving to another website), the session is discarded and all input data and results with it.

Despite these limitations, data storage on the server is possible, but depends on a number of prerequisites:

- generation and administration of user accounts;
- logon procedure to identify users, e.g. with user name and passwords;
- storage area (i.e. database) for depositing and recovering input data and results from emission estimations (data sets);
- option for data saving under a specific name to be entered by the user;
- extra dialog sequences for retrieving / selecting stored data sets;
- mechanism for the restoration of emission scenarios from stored data;
- mechanism for administrating stored data, e.g. to discard data sets not needed any more.

The efforts and resources involved for implementing such user accounts with permanent data sets surpass the scope of the current project which has its focus on demonstrating the feasibility and ease of tier-1 emission estimations according to REACH.

However, a full version for general productive use should definitely offer such an option later on.

8. Overall Architecture

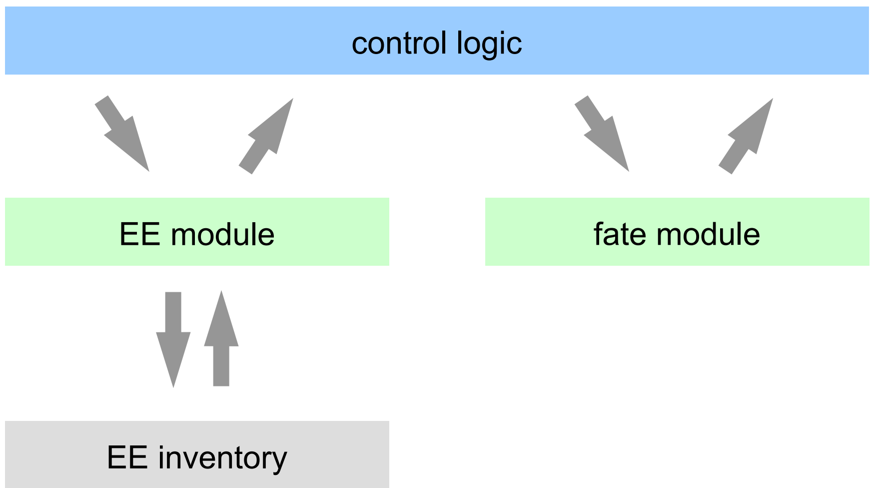
The aspects of the IT system introduced in chapter 7 are described in greater detail in this chapter.

Chapter 8.1 focuses on the central structural elements from a software developer's point of view.

Chapter 8.2 intends to provides a description of the logical sequence from the user's point of view. It is supplemented by the detailed "dialog sequence" described in annex I.

8.1. Server-based Implementation

The following graphic illustrates the interaction of the essential structural elements:



The control logic comprises the entire "intelligence" for running the program.

For the calculation of emission estimations the EmE module is called. This in turn retrieves the specific rules for the chosen emission scenario from the EmE inventory. The result of the calculation is returned to the control logic.

A subsequent optional fate modelling is processed by the fate module, which again returns a calculated PEC value to the control logic.

8.1.1 EmE Module

The EmE module will be generically programmed so it will be reusable. All emission estimations implemented in the prototype or future versions of the EmE tool will be carried out with the same EmE module.

With each invocation of the EmE module the control logic provides the necessary information which emission estimation is to be calculated. All information and rules required for this specific scenario is deposited in the EmE inventory.

Thus the EmE module does <u>not</u> contain programmed algorithms for the calculation but uses a set of rules to evaluate the relevant EmE inventory entries at run-time, this way composing the required calculation model for each individual emission scenario.

Therefore, EmE module and EmE inventory are both essential for each calculation of an individual emission estimation.

8.1.2 EmE Inventory

The EmE inventory stores all the rules and default values needed for each emission scenario. The following information is contained in the inventory:

- *calculation and look-up rules*
  The *rules* to be applied to perform the desired emission estimation.
- *emission parameters*
  The specific parameters needed to perform the desired emission estimation. For each parameter details are stored that control the input dialog for the user.

"Rules" can either refer to mathematical formulas or to look-up mechanisms to choose a value by superimposing input parameters with predefined look-up tables.

It is evident that the EmE inventory will *not* be able to store rules of unlimited complexity for the individual scenarios. Prior to the implementation of the EmE tool, conventions will have to be developed determining the degree of complexity that is expected for the emission estimations implemented within the scope of this project and later on.

8.1.3 Fate Module

Unlike the generic approach of the EmE modules the fate module will be programmed individually. A fate module will only be provided for the water path (⇨ chapter 5.5), but it should be applicable to all emission scenarios alike. The fate module works with aggregated values derived from A/B tables and therefore uses a simple mathematical model.

The fate module will be supplied with the input of relevant substance specific fate parameters from the input of General Information (⇨ chapter 8.2.2). Therefore, no extra dialog step is required for this module.

8.1.4 Control Logic

The central control logic is responsible for running all general parts of the program, i.e. those parts not dealing with specific emission scenarios. These comprise:

- Main menu
- Supply chain selection
- Input of General Substance Information
  (market data, substance properties, fate parameters)
- Selection of the life-cycle stage within the supply chain,
  or return to "Main menu"
- Navigation within selected life-cycle stages
- Execution of the appropriate EmE module
- Execution of the fate module
- Output of the resulting emission rate per day and PEC value
- In case of PEC>PNEC offering an iteration cycle with refinements
- Otherwise: return to "Selection of life-cycle stage"

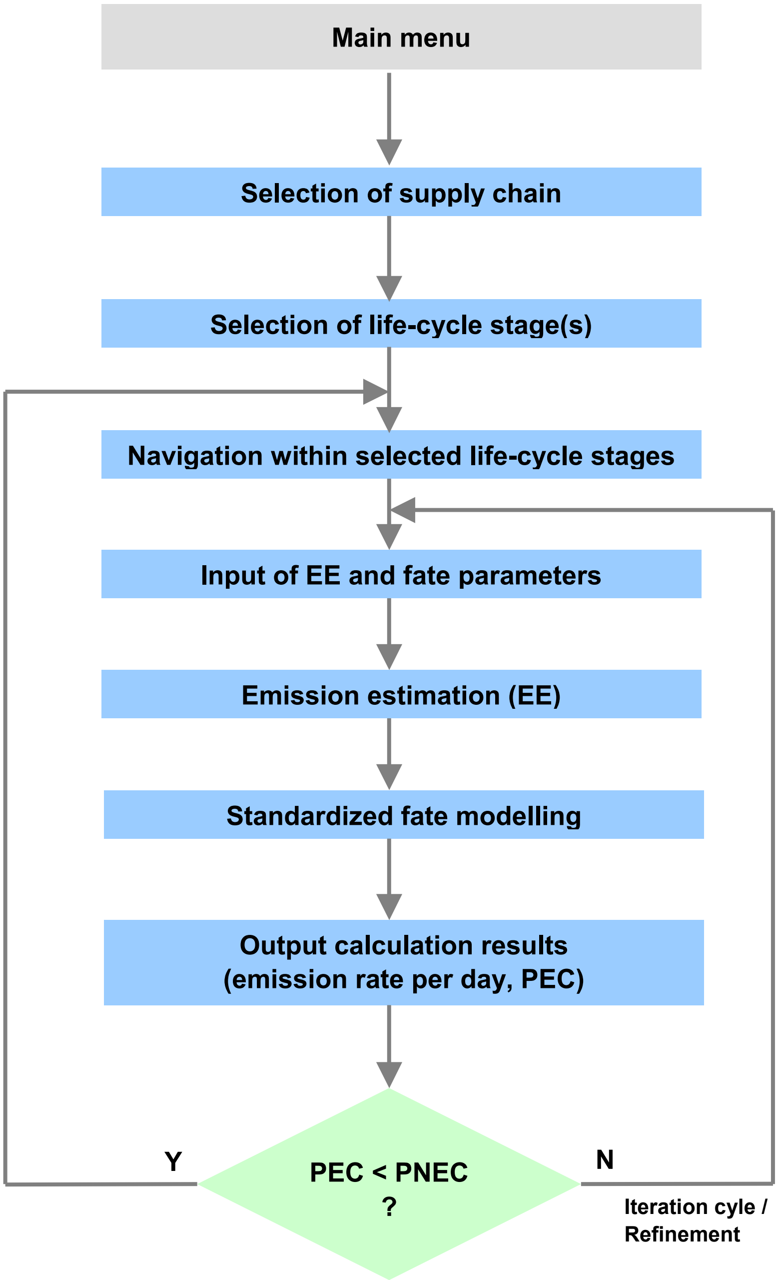
In addition, the control logic covers all requirements resulting from the IT-implementation as a web application, e.g. session management.

8.2. User Interface

The graphic on the next page shows all major elements of the overall user dialog. Its purpose it to provide a general overview, without going into greater detail of user dialogs.

The dialog steps and the relevant input items and resulting information are elaborated in detail in the user dialog sequence (⇨ annex I).

The main course of the dialog sequence is depicted in the following:


Main menu
Selection of supply chain
Selection of life-cycle stage(s)
Navigation within selected life-cycle stages
Input of EE and fate parameters
Emission estimation (EE)
Standardized fate modelling
Output calculation results
(emission rate per day, PEC)
Y
PEC < PNEC
?
N
Iteration cyle /
Refinement

8.2.1 Initial Steps

All steps in the logical sequence prior to the emission estimation are regarded initial:

In project phase A ("funnel project") a procedure has been developed for identifying relevant emission scenarios with the help of common classification schemes (⇨ chapter 5.2). It is intended in a later project to implement this procedure into a software application that can "feed" its result (an emission scenario) as a selection into the IT tool.

Currently the results from project phase A are directly applied (for the two supply chains covered) by sequentially asking for product chain and life-cycle stage. The ESD guidelines applicable for the selected combination are the basis for the underlying EmE module.

Selection of Product Chain

According to the current concept only few initial steps will be needed. The required product chain will be selected directly in the main menu. This is the starting point for each user calling the URL of the EmE tool in a browser.

Selection of Life Cycle Stages

Once the relevant supply chain has been determined, the user chooses one or more life-cycle stages of interest. With this choice, the user also determines his own role as stakeholder. If the user starts with the life-cycle stage "Industrial Use", he is considered an industrial user. This is important for certain parameters, e.g. which value to accept as "handled substance volume (Q)".

After each emission estimation the user will return to a dialog for the navigation within the *selected* life-cycle stages. Here, it will be possible to repeat calculations for the same stage, if other emission scenarios need to be considered parallel, e.g. in *service life*. However, the results of parallel scenarios will have to be summed up manually.

Alternatively, it will be possible to select the next *downstream* life-cycle stage or to repeat a previously calculated *upstream* life-cycle stage.

8.2.2 Emission Scenario

Input of General Information

The selection of a life-cycle stage corresponds to a set of specific predefined EmE modules (one for each environmental compartment).

This dialog step will comprise sequential input of all parameters needed for these particular emission estimations <u>including</u> the fate parameters for exposure estimation.

Calculation of Daily Emission Rate

Each life-cycle stage will be initially calculated with default values derived from ESD or TGD A/B tables. Therefore, extra input will not be required at this stage. After this, the calculation may be repeated with input values manually entered by the user, overriding the default values, in two increasingly specific iteration cycles.

The program will display the resulting daily emission rate <u>after</u> the calculation of the exposure estimation (⇨ chapter 8.2.3).

8.2.3 Exposure estimation

The calculation of an exposure estimation value (PEC) and its comparison is performed automatically in succession to the calculation of the daily emission rate, so no extra input step is required. All the necessary parameters have already been entered with the General Information (⇨ chapter 8.2.2).

Calculation of PEC

Using the previously calculated emission rate and the extra parameters entered as part of the General Information, a PEC value will be determined and automatically compared with the PNEC value (see below).

PEC / PNEC Comparison

The PEC/PNEC comparison is performed automatically and the result will be displayed directly afterwards.

With the display of the results an option will be offered to perform a more specific calculation (iteration cycle / refinement, see below).

Otherwise the user returns to the "Selection of Life Cycle Stage" (⇨ chapter 8.2.1) from here.

Iteration Cycles and Refinements

If the user has opted for a more specific calculation ("iteration cycle" / "refinement") as a result of an unduly high PEC, he will be guided back to the input of emission drivers (⇨ chapter 8.2.2). There he can repeat the calculation on the basis of the refined values and extended items.

The program sequence distinguishes between "iteration cycles" and "refinements"

- With each of max. three iteration cycles, extra specific items (e.g. STR, on-site emission reduction measures etc.) are presented, so that the user can influence these.
- Refinements offer the option to overwrite default values for certain emission drivers..

Annex I

Dialog Sequence

for the

Branch- and product-related emission estimation tool
for manufacturers, importers and downstream users
within the REACH-system ("IT-Tool")

IT Tool – Dialog Sequence for Emission Scenario "Plastic Additives"

Based on: "IT-Guidance "Plastic Additives", A. Reihlen, Oekopol Institute

Version of 31-Aug-2005

General Information

Emission Scenario

Dialog	Dialog type	Ref. IT-guid.	Remarks
selection of relevant EmS	selection (pick list)	chap-2.1	

Market data

own substance volume handled [t/a]	input	chap-2.2.2	
EU market volume [t/a]	input	chap-2.2.2	

Substance properties

vapour pressure [Pa]	input	chap-2.2.1	grouping in "high", "medium", and "low"
solubility [mg/l]	input	chap-2.2.1	
molecular weight [g/mol]	input	chap-2.2.1	
physical state	selection (pick list)	chap-2.2.1	
degradability range	selection (pick list)	chap-2.2.1	grouping according to STP module
log Pow range	selection (pick list)	chap-2.2.1	grouping according to STP-module
PNEC of the substance [µg/l]	input	chap-2.2.1	

Relevant life cycle stages

relevant life cycle stages	multiple selection / de-selection (pick list)	chap-2.2.3	

Selection of current life cycle stage

OBS.: Point of re-entry after execution of an emission estimation. Supports selection of a) the next downstream stage (default), b) repeated calculation of the same stage, c) repeated calculation of an upstream stage already calculated before.

Dialog skipped at the first emission estimation, i.e. after the pre-selection of "relevant life cycle stages" to be considered.

Selection of cycle stage for current estimation

Dialog	Dialog type	Ref. IT-guid.	Remarks
current life cycle stage	selection from list of predefined relevant life cycle stages	[---]	

Life cycle stage "production"

Iteration 1

Dialog	Dialog type	Ref. IT-guid.	Remarks
[not applicable]			see remark in chap-3.1

Iteration 1 – refinement

[not applicable]			see remark in chap-3.1

Iteration 2

emission days in production [d/a]	input	chap-3.1.1	no default value for production
results: E_{water}, E_{air}, E_{soil}, $PEC_{local+backgd}$, PEC/PNEC ratio	presentation of results and factors implicitly applied	chap-3.1.1	F_{air}, F_{water} and F_{soil} picked from table 7.1 in long version manual

Iteration 2 – refinement

share of wastewater discharged to municipal STP [%]	input (percentage)	chap-3.1.1	k_{STP} calculated via STP module
results: E_{water}, E_{air}, E_{soil}, $PEC_{local+backgd}$, PEC/PNEC ratio	presentation of results and factors implicitly applied	chap-3.1.1	F_{air}, F_{water} and F_{soil} picked from table 7.1 in long version manual, con factor applied (100% or 0%)

Iteration 3

share of waste gas treated on-site	input (percentage)	chap-3.1.2	
share emitted after on-site waste gas treatment	input (percentage)	chap-3.1.2	calculation: 100% minus efficiency of waste gas treatment
share of waste water treated on-site	input (percentage)	chap-3.1.2	
share emitted after on-site waste water treatment	input (percentage)	chap-3.1.2	calculation: 100% minus efficiency of waste water treatment
results: E_{water}, E_{air}, E_{soil}, $PEC_{local+backgd}$, PEC/PNEC ratio	presentation of results and factors implicitly applied	chap-3.1.2	F_{air}, F_{water} and F_{soil} picked from table 7.1 in long version manual, con (100% oder 0%) and F_{emred} factors applied

Iteration 3 – refinement

[not applicable]			

Life cycle stage "formulation"

Iteration 1

Dialog	Dialog type	Ref. IT-guid.	Remarks
results: E_{water}, E_{air}, E_{soil}, $PEC_{local+backgd}$, PEC/PNEC ratio	presentation of results and factors implicitly applied	chap-3.2.1	F_{air} = 1.025%, F_{water} = 0.675%, F_{soil} = 1%. T=20

Iteration 1 – refinement

[not applicable]			

Iteration 2

emission factor for raw materials handling	selection (table look-up)	chap-3.2.2	$F_{rawmat, air}$ and $F_{rawmat, water}$ picked from table 7.4 in long version manual
emission factor for compounding	selection (table look-up)	chap-3.2.2	$F_{compounding, air}$ and $F_{compounding, water}$ from table 7.5 in long version manual
results: E_{water}, E_{air}, E_{soil}, $PEC_{local+backgd}$, PEC/PNEC ratio	presentation of results and factors implicitly applied	chap-3.2.2	F_{rawmat} and $F_{compounding}$ added for water and air, respectively F_{soil} remains unchanged (1%).

Iteration 2 – refinement

only if tool started from an earlier life cycle stage: share used by main client *if tool started at current life cycle stage:* dialog step omitted	input (default override)	chap-3.2.2	replaces default value for Q or f, respectively
emission days	input (default override)	chap-3.2.2	replaces default value for T
share of wastewater discharged to municipal STP [%]	input (percentage)	chap-3.2.2	F_{STP} calculated via STP module
results: E_{water}, E_{air}, E_{soil}, $PEC_{local+backgd}$, PEC/PNEC ratio	presentation of results and factors implicitly applied	chap-3.2.2	F_{STP} applied to F_{water} calculation, F_{air} and F_{soil} remain unchanged

Iteration 3

share of waste gas treated on-site (con_{air})	input (percentage)	chap-3.2.3	
share emitted after on-site waste gas treatment	input (percentage)	chap-3.2.3	100% minus efficiency of waste gas treatment
share of waste water treated on-site (con_{water})	input (percentage)	chap-3.2.3	
share emitted after on-site waste water treatment	input (percentage)	chap-3.2.3	100% minus efficiency of waste water treatment
results: E_{water}, E_{air}, E_{soil}, $PEC_{local+backgd}$, PEC/PNEC ratio	presentation of results and factors implicitly applied	chap-3.2.3	F_{emred} applied to F_{water} and F_{air} calculation, F_{soil} remains unchanged

Iteration 3 – refinement

[not applicable]			

Life cycle stage "industrial use"

Iteration 1

Dialog	Dialog type	Ref. IT-guid.	Remarks
results: E_{water}, E_{air}, E_{soil}, $PEC_{local+backgd}$, PEC/PNEC ratio	presentation of results and factors implicitly applied	chap-3.3.1	F_{air} = 0.25%, resp. 99% for blowing agent (liquid or gas), F_{water} = 2.5%, F_{soil} = 10%, T=4.5

Iteration 1 – refinement

[not applicable]			

Iteration 2

emission factor for conversion	selection (table look-up)	chap-3.3.2	F_{air} and F_{water} picked from table 7.7 of long version manual
results: E_{water}, E_{air}, E_{soil}, $PEC_{local+backgd}$, PEC/PNEC ratio	presentation of results and factors implicitly applied	chap-3.3.2	F_{water} and F_{air} re-calculated, F_{soil} remains unchanged

Iteration 2 – refinement

only if tool started from an earlier life cycle stage: share used by main client *if tool started at current life cycle stage:* dialog step omitted	input (default override)	chap-3.3.2	replaces default value for Q or f, respectively
emission days	input (default override)	chap-3.3.2	replaces default value for T
share of wastewater discharged to municipal STP [%]	input (percentage)	chap-3.3.2	F_{STP} calculated via STP module
results: E_{water}, E_{air}, E_{soil}, $PEC_{local+backgd}$, PEC/PNEC ratio	presentation of results and factors implicitly applied	chap-3.3.2	F_{STP} applied to F_{water} calculation, F_{air} and F_{soil} remain unchanged

Iteration 3

standard RMM for waste gas treatment	selection (table look-up)	chap-3.3.3	applicable only to some additive types; ➔ still to be finalized
results: E_{water}, E_{air}, E_{soil}, $PEC_{local+backgd}$, PEC/PNEC ratio	presentation of results and factors implicitly applied	chap-3.3.3	F_{emred} applied to F_{air} calculation, F_{water} and F_{soil} remain unchanged

Iteration 3 – refinement

share of waste gas treated on-site (con_{air})	input (percentage)	chap-3.3.3	
share emitted after on-site waste gas treatment	input (percentage)	chap-3.3.3	100% minus efficiency of waste gas treatment
share of waste water treated on-site (con_{water})	input (percentage)	chap-3.3.3	
share emitted after on-site waste water treatment	input (percentage)	chap-3.3.3	100% minus efficiency of waste water treatment
results: E_{water}, E_{air}, E_{soil}, $PEC_{local+backgd}$, PEC/PNEC ratio	presentation of results and factors implicitly applied	chap-3.3.3	F_{emred} applied to F_{water} and F_{air} calculation, F_{soil} remains unchanged

Life cycle stage "service life"

Initial question

Dialog	Dialog type	Ref. IT-guid.	Remarks
Life cycle stage "service life" not applicable to: - *polymeric impact modifier,* - *curing agent,* - *coupling agent,* - *blowing agent (chemical),* - *viscosity aid*	Display of message, followed by an "abort" option	chap-3.4	

Iteration 1

Dialog	Dialog type	Ref. IT-guid.	Remarks
results: E_{water}, E_{air}, $PEC_{regional+backgd}$, PEC/PNEC ratio	presentation of results and factors implicitly applied	chap-3.4.1	F_{air} = 0.01, F_{water} = 0,032, E_{soil} not applicable

Iteration 1 – refinement

[not applicable]			

Iteration 2

product lifetime and emission factor	selection (table look-up)	chap-3.4.2	Air / water lifetimes, F_{air} and F_{water} picked from table
results: E_{water}, E_{air}, $PEC_{regional+backgd}$, PEC/PNEC ratio	presentation of results and factors implicitly applied	chap-3.4.2	F_{water} and F_{air} re-calculated, F_{soil} not applicable

Iteration 2 – refinement

prolonged water lifetime for specific product types	selection (table look-up)	chap-3.4.2	Prolonged water lifetime picked from table
results: E_{water}, E_{air}, $PEC_{regional+backgd}$, PEC/PNEC ratio	presentation of results and factors implicitly applied	chap-3.4.2	F_{water} re-calculated, F_{air} remains unchanged, F_{soil} not applicable

Iteration 3 / Iteration 3 - refinement

[not applicable]			

Life cycle stage "waste"

Initial question

Dialog	Dialog type	Ref. IT-guid.	Remarks
Life cycle stage "service life" not applicable to: - *polymeric impact modifier,* - *curing agent,* - *coupling agent,* - *blowing agent (chemical),* - *viscosity aid,* - *anti-static agent (organic)* - *blowing agent (solid)* - *slip promoter (organic)*	Display of message, followed by an "abort" option	chap-3.5	

Iteration 1

Dialog	Dialog type	Ref. IT-guid.	Remarks
results: E_{water}, E_{air}, $PEC_{regional+backgd}$, PEC/PNEC ratio	presentation of results and factors implicitly applied	chap-3.5	all emissions from production, formulation and industrial use, plus 100% of substance remaining in final products; ➔ still to be developed

Iteration 1 – refinement

results: E_{water}, E_{air}, $PEC_{regional+backgd}$, PEC/PNEC ratio	presentation of results and factors implicitly applied	chap-3.5	➔ still to be developed