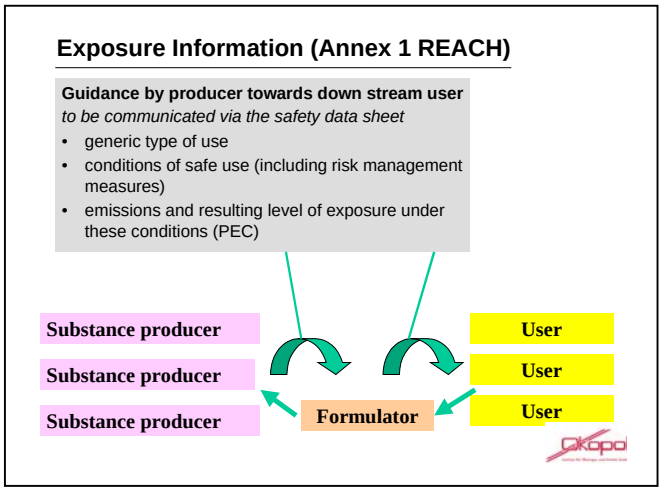
Co-operation in the development of REACH-Tools

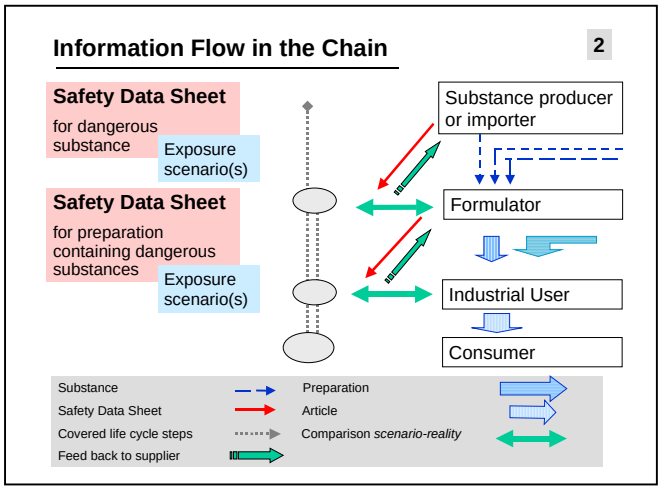
Screening tool supporting environmental exposure assessment under REACH for substances used in textile finishing

Short Project Report[1] (December 2004)

1. Background

Under the REACH system as proposed in the draft REACH regulation (October 2003) companies importing/producing and marketing of substances > 1 t/a are obliged to register these substances. For dangerous substances in quantities exceeding 10 t/a, a chemical safety assessment (including exposure assessment) is required. The exposure assessment comprises (an) exposure scenario(s), including generic type(s) of use and conditions of use, and a prediction of the level of exposure to be expected. The exposure assessment needs to cover all life cycle steps from manufacturing of the substance and formulation of the preparation down to the use of the preparation in manufacturing of articles and the service life of these articles. All environmental compartments and each population likely to be exposed (e.g. worker, consumer) shall be covered for every life cycle step. This paper is focussed on safety assessment related to the environment.





At least three stakeholders in the supply chain need to contribute information to the safety assessment.

- The substance producer provides information on
  - the substance properties (hazard and exposure relevant),
  - the conditions of use (including risk management) he believes to be safe
  - and a comparison between the estimated level of exposure that could occur under these conditions and the level of exposure at which no adverse effects are anticipated to occur.
- The formulator provides information on
  - the percentage of dangerous substance in his preparation,
  - possibly more specific information on the type and conditions of use,
  - and based on this, possibly more specific emission factors and exposure estimates.

[1] R+D project sponsored by the German Federal Environmental Agency (UBA); FKZ: 202 67 433

- The industrial user of the preparation contributes information on
  - daily amounts used at a certain site and the frequency of use
  - the capacity of the environment to dilute the emission (including municipal wastewater streams)
  - and possibly more specific information on the type and conditions of use (including the measures for pollution prevention and control).

Only a combination of all this information leads to a realistic chemical safety assessment. However, practical implementation of such a concept meets various challenges. Based on the experience gained in a REACH simulation carried out in North-Rhine-Westphalia[2] the difficulties can be summarised as follows:

- The three actors in the chain do not use the same "language";
- The information is partly not meant to be disclosed towards suppliers or customers;
- The information needs to be structured and processed in a way that the assessment can be done with minimal efforts in the majority of cases:
  - Categorisation of use and exposure patterns in order to allow for standard-phrases and to ensure sufficient flexibility for innovation with regard to types and conditions of use;
  - A tiered system that allows for sequential conclusion whether further or more detailed information is needed;
- A harmonised IT-system to generate and communicate the information across the EU market is needed.

In order to develop a workable system, a set of generic exposure scenarios (including standard risk management options) is needed, under which the great variety of use and exposure patterns in the market can be clustered. An example of the development of such a chain-specific generic scenario involving various stakeholders is outlined below.

2. Objectives of the project

The current project aimed to develop a generic exposure scenario (including a tool for calculation of exposure concentration) for the use of dye stuffs and finishing chemicals in the textile manufacturing sector. This scenario is structured in such way that it may serve as a prototype for other sectors as well. The exposure scenario and the exposure estimation were integrated into an IT-tool to be used at company level.

The current concept has been worked out by an ad-hoc working group consisting of 3 textile finishers, 3 companies manufacturing textile chemicals, the German Federal Environmental Agency (UBA), 3 associations (representing textile manufacturers, textile finishers and producers of textile finishing chemicals) and a group of consultants (list of participants see attachment 1). The exposure scenario and the exposure estimation tool at the current stage of development should be understood as an illustration how exposure assessment and communication in the supply chain may work under REACH. The working group hopes that it has worked out a useful contribution to the upcoming *REACH Implementation Projects* (RIP) number 3.2 and 3.5.

[2] Testing of selected elements of the REACH procedures in practise by authorities and companies in North Rhine-Westphalia (Germany); summary project report 22.12.03; www.europa.nrw.de;

3. Basic Scenario

In a first step, a basic scenario was defined: Discharge of water-soluble substances (WS > 1 mg/l) to surface water via a biological wastewater treatment plant (WWTP) from a textile finishing company. The WWTP is regarded as the standard risk management measure, and the water compartment is regarded as the standard receiving environment.

In addition, some other relevant emission pathways and environmental compartments at local level were identified and addressed in the generic scenario:

- discharge of poorly water-soluble and/or adsorptive, organic substances to surface water including potential exposure of sediments, agricultural soil (via sewage sludge) and biota (via secondary poisoning): For these compartments, the exposure estimation tool does not yet provide a quantitative exposure assessment.
- air emission related to textile finishing through foulard/padding and printing processes (including air scrubber as the standard risk management measure).

External waste treatment has not been addressed in the current project. Also, the other life cycle stages (production of substance, formulation of preparation and the substance service life in articles, waste disposal) have been set aside for the time being. The same applies to the regional scenario.

4. Identification of factors driving the exposure

Based on the OECD Emission Scenario Document (ESD), the EU Technical Guidance Document on Risk Assessment for New and Existing Substances (TGD) and the practical experience of the companies involved, five main factors have been defined: Each of the factors has been assigned to that actor in the chain most likely to have access to realistic, site or substance specific information (e.g. substance properties – producer; quantity used at a certain site – down stream user). In order to allow for an exposure estimate at another level (e.g. producer's assumption on site specific quantity at user's level) default values have been defined that can be overwritten with more realistic information whenever this becomes available.

- **Exposure relevant substance properties**: The substance producer usually knows (or determines) the relevant substance properties, i.e. water solubility, vapour pressure, octanol-water partition coefficient (Log K_{ow}), biodegradation and molecular weight. These parameters should be available and hence no defaults need to be defined.
- **Losses of substances during textile dying and finishing**: There are two general cases, either the substance is made for uptake onto/into the fabric (e.g. dyes, optical brighteners, softeners), or it is a textile auxiliary remaining in the water e.g. detergents (100% to wastewater). Although, many dyes and textile finishing chemicals fix to the fabric at a degree of more than 90%, a default of 70% is assumed in order to also cover textile finishing chemicals and residues from foulard dipping baths and printing processes.
- **Used amounts per time and frequency of use:** Usually the producer of a substance does not know the daily amount of a substance (contained in a textile finishing preparation) used at a certain site (local scenario). Furthermore he does not know whether the substance is used continuously or only from time to time (e.g. not more than 1 day per month). Hence the producer will make a default assumption for his exposure estimate, e.g. 150 kg/day and daily use. The textile finisher can replace the default value by more realistic values.

- **Elimination in biological wastewater treatment**: The biological elimination in a wastewater treatment plant depends on the biodegradability of the substance and the partitioning of the substance between sludge, air and water in the wastewater treatment plant. In the present type of assessment, results from OECD standard screening biodegradation tests (OECD 301 A-F and 302 B-C) and the *SimpleTreat* model (see TGD) are used to determine the elimination rates and the need to consider a sludge scenario. In order to keep the work focussed, air emission from wastewater treatment and potential sludge respiratory inhibition have been set aside for the time being.
- **Dilution in relevant environmental compartments:** Again the producer does not know the relevant receiving water volume (wastewater and surface water) available to dilute the releases from wastewater treatment. Based on the TGD a default of 20.000 m^3/d is used (dilution of 2.000 m^3/d wastewater by factor of 10), which again can be replaced by more realistic figures for the local situation.

The approach outlined above would also allow for setting up bands (categories) for substance amounts and dilution volume, if this would further simplify the task for the actors in the supply chain.

5. Quantitative exposure assessment

During the scenario development, quantitative exposure calculation and comparison with the relevant Predicted No Effect Concentration (PNEC) was carried out by means of an excel spreadsheet. The spreadsheet contains a default value for each parameter[3] and an option to overwrite the default value with more realistic information. If the following defaults for emission of a water soluble substance (biodegradability not demonstrated) via wastewater are used, a default PEC of 7.5 mg/l (100 % loss) results.

- Amount of substance used in a textile finishing company per day 150 kg (Draft ESD, 2003)
- Losses to wastewater 100 % (if substance is not intended to be up-taken onto/into the fabric) or 30 % (reasonable worst case if substance is intended to fix to the fabric; based on industry information)[4]
- Elimination factor for substance for which ready or inherent biodegradability is not demonstrated: 0 %
- Volume of receiving local wastewater and river water: 20.000 m^3 /day

For many substances and conditions of use, the PEC is most likely significantly lower if more realistic values are used instead of the defaults. All three actors can contribute information available to them to screen out those conditions of use, for which in fact no further assessment is needed. For example, the daily amount is possibly not higher than 25 kg, the substance has turned out to be inherently degradable[5] and the available water volume for dilution is 2 million m^3/d instead of 20.000 m^3/d. In such a case the PEC would be 7.5 µg/l (still

[3] The default values for elimination in WWTP are derived from the tables given in Appendix II of Chapter 3 "Environmental Risk Assessment" of the TGD. Values are rounded.

[4] In some cases, for example fabric softeners, the technical function of the substance is only to remain in the fabric until the first washing by the private consumer. 100% release of these substances would be addressed in a regional scenario.

[5] Based on the S*impleTreat model* the biological elimination of a water soluble, non-volatile organic substance in waste water treatment would be about 40% . Accordingly, the discharge of losses to surface water is 60% instead of 100%.

100 % losses to wastewater assumed). Any substance with an acute toxicity > 7.5 mg/l could be safely used even without further assessment of the degree of fixation to the fibre. However, the manufacturer of the substance would need to state in his exposure scenario that safe use is only ensured if the daily amount does not exceed 25 kg and the receiving water volume is not below 2 million m^3 per day.

6. Refinement of information if PEC > PNEC

If this first cycle of safety assessment still leads to a concern (PEC > PNEC) the tool provides some guidance for a second safety assessment cycle with more specific and more realistic information. In many cases for example, a dye may fix to the fabric to a degree of 95% or the residues from the foulard dipping baths are minimised to 5% instead of 30%.

Only if this second round of safety assessment still ends with a concern, a further assessment on a case by case basis is needed.

7. Points of discussion related to the risk assessment methodology

During the scenario and tool development, a number of scientific questions related to exposure assessment were to be clarified:

- The water-octanol partitioning coefficient (log Pow) could be a misleading predictor for adsorption in case of surface active and/or ionic substances. Hence an indicator had to be defined when modelling based emission estimate (*SimpleTreat*) may or should be replaced by a measured log Koc or by adsorption measured in a Zahn-Wellens-Test (OECD 202-B).
- For detergents, the 10 day window in the OECD screening on ready biodegradation does not apply. According to SCHER (formerly CSTEE) these substances are regarded readily biodegradable if they reach the pass level in a 28 days study even when failing to meet the 10 day window criterion[6].
- In the textile finishing sector, the results of OECD 302 B test are often used to determine ***elimination*** (degradation plus adsorption) of substances in biological wastewater treatment. In the current safety data sheets, this is often expressed as 90% elimination or more. However this approach has not been used in the current exposure estimation tool since the REACH proposal includes a ready biodegradation test and the log Pow as a standard information requirement. The percentage of substance eliminated from wastewater should be determined based on the S*impleTreat* model in the TGD as the standard approach. However, if the log Pow is not applicable, the adsorption control in OECD 302 can be used to measure adsorption to sludge.

8. Air emission scenario

Emissions to air from padding processes can be relevant in the textile finishing industry. At temperatures between 120 and 240 °C substances from textile finishing chemicals, dye carriers as well as spinning oils (processing aids from pre-processes) may be emitted from the fabric.

The emissions contain substances (as defined in the chemicals legislation) and various metabolites being generated in the process. The current scenario only addresses the “sub-

[6] According to "OECD Guideline for testing of chemicals: 301 Ready Biodegradability", the pass level of 60% or 70% mineralisation has to be reached within 10 days after the degradation process has entered into its logarithmic phase (point in time when 10 % degradation is reached).

stances" as such based on the German „Bausteine-Concept"[7]. In the first exposure assessment circle 100 % losses to air and no emission control is assumed. The local PEC is determined based on the TGD. In a refinement cycle, a substance specific emission factor can be used (if available) and emissions are reduced by air scrubber.

9. Translating the concept into an IT-tool (MS ACCESS Application)

The concept of a generic exposure scenario (including a tool to estimate the level of exposure) has been integrated into a MS *Access*© application. Even though the excel spreadsheet may be sufficient in terms of simple emission and exposure calculation, the MS *Access* application adds further elements to the tool:

- Decision support for determining the need to carry out an exposure assessment under REACH
- In the *Access* data base, substance or product related data sets can be stored.
- The user interface supports guided assessment loops and the explanation for each step of the assessment procedure.
- Due to its modular set-up, additional life cycle stages or environmental compartments can be integrated into the system step by step.

The access application contains the following components (see also screen shots in attachment 2). Each actor in the supply chain uses the same data model to store his data-sets. Hence the information available to each level of the supply chain can be entered into a shared safety assessment.

(a) identification of supply chain level (producer, formulator, finisher), substance identity, name and type of preparation, generic type of textile finishing process

(b) decision tree to establish whether exposure scenarios have to be defined under REACH. This includes an evaluation whether sufficient information is available to carry out hazard classification.

(c) a table to insert the core environmental fate parameters of the substance including a question whether emission to water and/or air can occur. Based on this table, the program highlights which emission pathways (air or water), compartments (water, sediment, soil/sewage sludge, biota) and assessment approaches (PBT or vPvB assessment) need to be taken into account.

(d) a series of systematic questions to insert the information needed to determine the local PEC_{water}

(e) comparison of PEC local with PNEC with the result of i) further information or additional measures needed or ii) no concern.

(f) options to take into account sporadic use of a substance (PNEC x 10) or adsorption to sediments (PEC x 10)

(g) an option to modify the results of *SIMPLE Treat* in cases where the LogPow may be a misleading predictor for adsorption.

(h) a number of popup windows that highlight the need to carry out further assessment related to agricultural use of sewage sludge and/or secondary poisoning.

(i) guided refinement cycle to reduce the substance losses to waste water

(j) a series of systematic questions to insert the information needed to determine the local PEC_{air}

(k) comparison of PEC local to DNEL (or PNEC if available) with the result of i) further information or additional measures needed or ii) no concern.

[7] Guideline to predict specific substance loads and Corg loads (amount of organic substances in air measured as carbon content) from fabric finishing chemicals at temperatures between 120 °C to 220 °C in padding process. The German formulators of textile finishing chemicals communicate specific emission factors to their customers for those organic or inorganic substances for which regulatory thresholds exist in Germany.

10. Reflections on the development process

The working process resulted in a generic exposure scenario for the use of substances in textile finishing. This may be applicable to other supply chains or group of actors as well. The characteristics of the process:

- In the project, all three levels of the supply chain were represented by single companies and by their associations.
- The OECD *Emission Scenario Document* and the TGD were taken as a starting point in order to ensure consistency with internationally agreed approaches. However, during the discussion it turned out that not all involved companies were aware of the existence of the *Emission Scenario Document* for the textile chain. Also, they were not familiar with the TGD. For the success of the further development process it was important to leave sufficient room for emerging ideas and to use the ESD and TGD in a flexible manner.
- Three of the five workshops were held at production sites representing different types of the finishing processes. It turned out to be very fruitful to connect the work on a generic (non-process-specific) tool with practical insight into the technical processes. This included e.g. comparing the assumptions on substance losses, pollution prevention and control measures and release factors with the practical experience of the involved companies.
- It was also particularly useful that one of the members of the project group had been working for several years with various textile finishers on pollution prevention and control, and hence had a broad overview on the state of the art of pollution control in the sector.
- The participation of the Federal Environmental Agency (UBA) in the working process was important. First of all, a constant feedback given by the Agency ensured that the result of the work stayed within the band of solutions acceptable to the authorities. Secondly, the participation of UBA was a clear signal to industry that also the Agency has an interest in searching for solutions simple enough to work out in practise.
- The translation of the generic scenario into an IT-tool was a good motivation to precisely think through the relevant assessment steps. At the same time, the IT-tool made the REACH concept of *exposure scenario* and *exposure estimate* touchable, thereby facilitating an increase of acceptance among the participants.

11. Proposals for further work

The project group believes that the results of the current project should be fed into the REACH Implementation Project 3.2 (Guidance on Chemicals Safety Report) and 3.5 (Down stream user requirements). The outcome of the current project may be seen as contribution for getting a common understanding how to implement the exposure assessment under REACH in practise. Beyond that, the current tool may be tested in other supply chains with a comparable pattern of emissions.

For further development of the concept, the following points seem to be important:

- How to connect the various systems for categorisation (classification) of exposure and uses with a generic exposure scenario for a supply chain.

- Should the algorithm calculating the level of exposure resulting from certain risk management measures become an element of the exposure scenario? According to REACH Annex I, the exposure scenario defines the safe conditions of use, whereas the exposure estimation is a separate second step. In order to link these two steps in a flexible way, the exposure scenario should include an instrument to calculate the exposure resulting from different options to prevent and control emissions. It would be on the formulators and users to calculate the level of exposure based on realistic figures.
- Compilation of a standard catalogue on measures for reduction of emission (based on current practise) and derivation of quantitative abatement factors.
- Add components on the life cycle stages „manufacture“, „formulation“, „use of textile“ (service life) and „waste disposal“
- Add quantitative elements for addressing the „soil compartment“ (via sewage sludge and air), the "air" (via wastewater treatment) and the "secondary poisoning through the food chain";
- Add a regional scenario
- Define the interface to consumer exposure scenario
- Define the interface to the occupational exposure scenario
- Develop a concept for data import and export

12. Concluding remarks

It is hoped that the outlined approach is workable and may help to screen out the majority of cases of “no concern” in a relatively simple way. For further information or comments please contact:

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Attachment 1 – Participants

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