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# Chemical Safety Assessments under REACH

The Chemical Safety Report under REACH documents how risks of chemical substances are to be controlled. **Froukje Balk** and **Leo van der Biessen** of **Royal Haskoning** share their experience

During 2009 and 2010, we were repeatedly invited for presentations on Chemical Safety Assessment (CSA) under REACH. As consultants for Royal Haskoning, we also prepared REACH dossiers for our clients on High Production Volume (HPV) chemical substances for which safety had to be demonstrated in all identified uses and during all phases in the life cycle.

Before REACH, this process was termed 'risk assessment' and it was part of well-known EU legislation for new and existing chemicals, biocides and plant protection products. A risk assessment was carried out under the responsibility of the authorities and industry could be involved.

Within REACH the responsibilities have shifted and the registrant, either manufacturer or importer (M/I), is in charge of the process which is now known as Chemical Safety Assessment/Chemical Safety Report (CSA/CSR). In this process, safety can be demonstrated through proving the absence of hazard or by comparing exposure with no effect levels. The creation of a REACH dossier requires the following steps, among others:

- Setting the stage
- Collecting or creating hazard data
- Determining the hazard & risk
- Refining risk assessments
- Implementing safety instructions

## Setting the stage

Under REACH, the M/I is obliged to register his substances produced or

imported over 1 tonne/year and submit a dossier to ECHA. The data requirements depend on the tonnage involved, with more physico-chemical properties, environmental fate and toxicity data being required in the dossier as this increases. For each substance that an M/I produces and/or imports at a volume above 10 tonnes/year, a narrative description of the hazards in a CSR is obligatory.

A special feature of REACH is that all available hazard data has to be shared. For toxicology data on vertebrates the use of existing data is mandatory, if the quality is good. Vertebrate testing is only allowed when no existing data is available and ECHA has agreed to the performance of the test.

Mandatory cooperation between producers and importers of the same substance in a Substance Information Exchange Forum (SIEF) and the voluntary formation of consortia interested in a group of related substances required a lot of attention, effort and time. The formulation of iron-clad contracts, substance identification and sameness discussion were the most bothersome aspects of this.

Cooperation between parties that are usually competing on the same market under the stringent EU competition and anti-trust laws proved cumbersome. For the front-runners, these negotiations started early 2007 when REACH was in place. For others, they continued until well into 2010.

Only after the conclusion of the contract could the actual work on preparation of the REACH registration dossiers start. In most cases, consortia were formed, with the members performing the majority of industry's work. Subsequently the results were shared in the SIEF under the conditions of a SIEF agreement.

Contract laboratories and consultants were preparing as well. They understood better than many of their industrial partners the volume of work that needed to be carried out after the contract discussions were finalised. The collection of acceptable data to prepare the dossier is no simple task. All data delivered by the contract partners are to be evaluated for completeness, quality and data ownership and the financial reimbursement value must be established.

During the various conferences in 2009 and 2010, we expressed our concerns that the workload for 2010 would be characterised as a 'tsunami'. And that is precisely what happened. A few proactive M/Is were prepared well ahead of the deadline, but for the majority 2H 2010 turned out to be extremely stressful.

## Hazard data

When consortia and SIEFs finally started to cooperate, hazard data were listed in spreadsheets. After evaluation of the data sources and quality, a first data gap analysis often showed that additional testing was

needed in all sectors, i.e. the required physico-chemical data, environmental and toxicological information was incomplete.

To prevent testing, read-across from available data for structurally related chemicals is an alternative. Major efforts are generally needed to demonstrate the validity of a read-across input, so the validity of the surrogate data may be disputed during later checks by the authorities.

The safe solution is to obtain the requested information by actually performing the study. Read-across may also lead to lower limit values, as the uncertainty is somewhat greater. Within a consortium this means that agreement must be reached on contracting out and monitoring laboratory studies.

Another possible way to fill data gaps is to request the waiving of a data requirement based on the absence of exposure or on the fact that the information was not needed to demonstrate the safe use of a substance. However, this solution is not applicable to all data requirements.

The last option is the preparation of a testing proposal, mandatory for testing related to the higher tonnage levels. Before the deadline on 1 December 2010, this was seen as an attractive way to postpone testing and still remain in business. Now, however, these registrants are facing the costs for the proposed tests and, maybe even more importantly, the implications when the results of the studies are used to evaluate safety further.

## Communication channels

If, based on the hazard data, a substance is classified as dangerous for a listed set of hazard classes or categories set out in Annex I to Regulation (EC) 1272/2008 or is assessed as a persistent, bioaccumulative and toxic (PBT) or a very persistent, very bioaccumulative (vPvB) substance, the CSR with the hazard descriptions is to be completed with



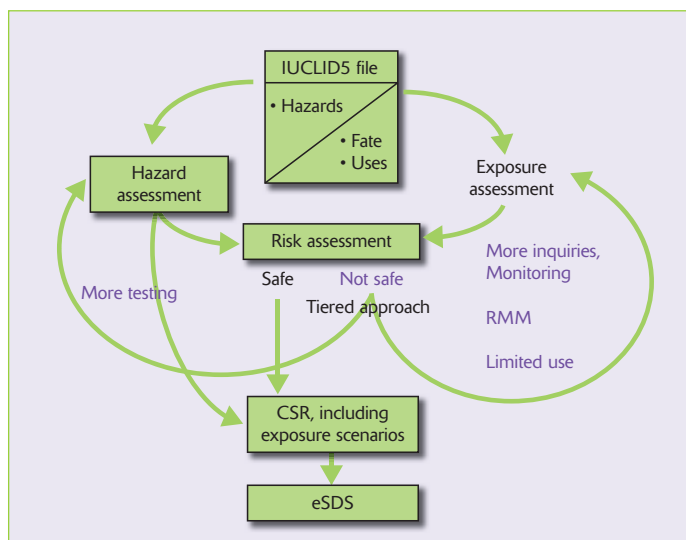


Figure 1 - Preparation of a CSR

an exposure assessment and risk evaluation covering its entire life cycle.

During the discussions preceding the adoption of REACH, the identification of all downstream uses of a substance was already recognised as a challenge. The level of detail needed for a realistic exposure assessment was to be balanced against the aspiration to create large use categories, with a view to effective communication of safety instructions down the supply chain.

ECHA guidance presents a use descriptor system based on a combination of life cycles stages (from manufacturing to end-use) and main user groups (industrial workers, professionals or consumers). Under each life stage the activities are identified and described in workers and consumer activities, some 30 process categories (PROCs) for workers and 40 chemical product categories (PCs). For each stage, one of 24 environmental release categories (ERCs) is assigned.

Identifying the best fitting categories requires not only sufficient expertise in the fields of occupational and environmental hygiene, but also in-depth knowledge of the applications by downstream users and their clients, as well as their operational conditions and risk control measures. This may cause problems when downstream users hesitate to deliver confidential information on specific uses. Thus the information received will be very general nature, allowing for only a very generic exposure assessment based on default parameters and resulting in 'realistic worst case assessments'.

Where supply chain communication has been a tradition for a long time, for example in the soap and detergent, paint and oil industries, industry associations have cooperated to produce higher level occupational and consumer exposure models and specific descriptions of the environmental release in various life cycle stages. These approach the actual practice in the industry and additional control measures beyond those already in place are only rarely needed.

#### Initial exposure assessment

In REACH terminology, an exposure scenario (ES) describes the conditions under which the risks associated with the identified use(s) of a substance can be controlled. This includes both operational conditions and necessary risk management measures. An ES is the result of an iterative risk assessment where relevant parameters determining the hazards and exposure are repeatedly refined, to conclude on the conditions where exposure to the substance will not exceed hazardous levels (Figure 1).

Where only generic information was delivered on the identified uses, the result of the initial risk assessment, Tier 1 presents a 'realistic worst case'. If the initial assessment demonstrates that the risks are controlled, this ES is transferred to the CSR.

The European Centre for Ecotoxicology & Toxicology of Chemicals (ECETOC) and ECHA have produced tools to carry out a Tier 1 risk assessment. The ECETOC Tiered Risk Assessment model is even integrated into ECHA's Chemical Safety Assessment & Reporting (CheSAR) tool.

These instruments can be applied without much expertise in toxicology or risk assessment but making the correct choices requires some skill. Annex I of REACH determines that the CSA shall be prepared by one or more competent person(s) who have appropriate experience and received appropriate training, including refresher training. The term appropriate is not defined, but logic dictates that the instruments used determine the skill required.

CheSAR produces output in the form of a CSR which can be inserted into the IUCLID dossier with a relatively limited amount of fine-tuning, typically taking a trained worker one or two days. From a practical point of view, this is very relevant because, even for a substance with a relatively simple life cycle (less than 100 identified uses or process steps), the exposure and risk assessment chapters in a CSR easily fill 300 pages. An exposure and risk assessment of more complicated substances can require several thousands of pages.

#### Refined risk assessment

The chances are that, for hazardous substances used in high production volumes, the Tier 1 assessment would indicate concern and refinements are needed. In the Tier 1 assessment tools, the exposure assessment can be refined by the introduction of additional measures to reduce the exposure, e.g. the use of closed systems, room ventilation or respiratory protection for workers, or of improved technology to reduce emissions or a mandatory reduction of the use volume on site for environmental protection.

In view of the burden on workers to use respiratory protection and the legal obligation to use personal protection equipment only as a last resort or the commercial implications of a reduction on use volume, this type of measures will not always be first choice. A better approach is to apply risk management measures only after higher tier models have been used to predict exposure.

A range of models is available to improve the occupational and consumer exposure predictions, whereas the predicted environmental exposure could already be refined considerably by an improved estimation of the fractions of the production volumes that are released to water and air. Other improvements

may be obtained, e.g. by realistic modelling of wastewater treatment and replacement of default dilution factors.

Finally, a verification of the predictions based on actual measurement of the exposure does not seem to be attractive to our clients, yet it may be a short cut to many modelling efforts and long discussions with the authorities. A refinement of the predicted exposure level could span several orders of magnitude. The application of these refinements requires a high level of expertise, generally available only in the larger industries and in specialised consultancy firms.

In many cases existing data from earlier measurement programmes were available. Unfortunately, most of this data was not usable, due to major errors in the measurement protocols, insufficient information on operational conditions and other reporting errors. For workplace measurement the minimal requirements are laid down in European Proposals for Core Information for the Storage and Exchange of Workplace Exposure Measurements on Chemical Agents.<sup>1</sup>

#### 'Worst case' assumptions

The 'worst case' approach is applied not only for the exposure estimation. For the environmental hazard assessment, safety factors of up to a factor of 1,000 are applied to the lowest aquatic toxicity values to derive a Predicted No Effect Concentration (PNEC). Chronic toxicity data that allow the use of factors of 50 or ten are rarely directly available.

If more results become available from additional testing, this does not automatically mean that the PNEC will increase: the value of the lowest toxicity level might decrease more than can be compensated for by the lower assessment factor. So additional testing does not automatically reduce the PNEC, though it does reduce the uncertainty about it.

A similar reasoning is valid for the Derived No Effect Level (DNEL) for human health protection. Yet, where a change could be in the order of a factor of five in an environmental hazard assessment, an improved estimate of the exposure can easily bring about a change of orders of magnitude.

Thus, where the results of an initial risk characterisation seem to identify a high concern, one should not immediately define the application as a 'use advised against' or to introduce stringent risk management

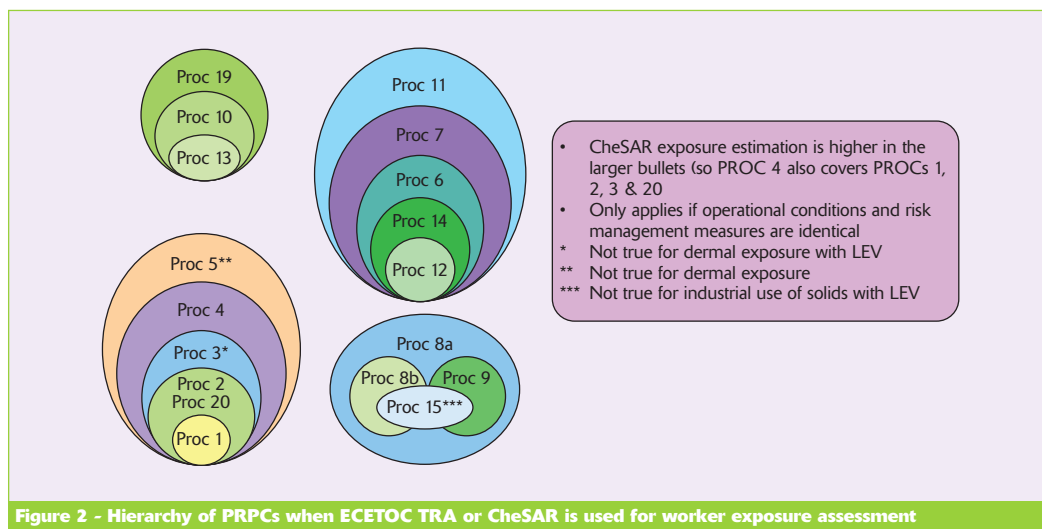


Figure 2 - Hierarchy of PRPCs when ECETOC TRA or CheSAR is used for worker exposure assessment

measures. Instead, a systematic consideration of the basic data on the hazards and, in particular, of the assumptions used to estimate the exposure should be performed to determine whether there are still realistic possibilities to lower the exposure to a safe level.

### Use of CSR results

Once a CSR with both a hazard and a risk estimate has been created, the M/I has to establish that he uses the substance as described. The information also needs to be integrated in the extended - or enormous! - safety data sheet (eSDS). Industry is still struggling with this task as an eSDS book of 2,000 pages without a proper index only conveys data instead of information.

Moreover, the appendix to the eSDS also needs to be supplied in all the relevant European languages. The current work on a European library of phrases (EUPHRAC) and the proposed generic exposure scenario (GES) tool seem to be the most promising at the moment.

The need to provide adequate information is enhanced by the fact that any use not included in the scenarios in the CSR is forbidden unless safety is established through a separate risk assessment. Scaling and bridging may be used as tools for such an assessment. The grouping of PROCs into hierarchies is another (Figure 2).

### It ain't over 'til it's over

Registering actually seems to be the easy part of REACH. Once a dossier is filed, the registrants cannot lie back. If the dossier contained testing proposals, they will need to perform the tests in time. The results may trig-

ger adaptations of the hazard and risk assessment.

Moreover, changes in legislation, guidelines or tools need to be evaluated in order to determine if the CSA/CSR or even the dossier require adaptation. Enquiries by later registrants, of other or similar substances, or data holders may be made and will need to be responded to in due course.

The hazard and risk data is to be distributed down the supply chain. Formulators need to extract and combine the relevant information from the eSDSs into their own SDS. The staffing of the SDS departments of formulators will be crucial and probably insufficient the coming years. And, if your substance winds up the Candidate List of Substances of Very High Concern, even article producers and suppliers will face major responsibilities in communicating the information.

### Recommendations for 2013

For all parties concerned, the 2010 'chemicals tsunami' was an exciting experience with a steep learning curve. By sharing our knowledge we hope to prevent a similar experience in 2013. The following are some of the key points.

First, the creation of a full dossier requires a lot of time. Both hazard and risk information is not readily available. If your SIEF is not active yet, get it started now.

As exposure models tend to overrate exposure somewhat, measured exposure can be helpful but be sure to have a valid report. Model a few of the most critical ESs now, so ample time is available to generate new data if necessary.

Once the dossier is prepared, information needs to be shared. Get your IT department familiar with the data tools

available (EUPHRAC and GES) and integrate them into your IT systems.

Especially in the first seven months of 2010, the production of new guidance documents by ECHA and industry exceeded everyone's capacity to absorb the information. This led to a moratorium in guidance publication. Another wave of guidance documents is expected in 2011-2012. These need to be digested and used for the 2013 registration and 2010 updates.

In April 2010 a beta version of CheSAR was made available. It was far from complete and it contained many fatal bugs. With much will power and perseverance we managed to produce basic CSRs using this tool that had to be checked and completed manually.

Even so, in view of the hundreds of pages resulting for assessments on relatively simple life cycles, we are happy we continued using CheSAR, as there was no equivalent alternative. It is vital to our services that ECHA improves the functioning of the tool and we will contribute as well as is reasonably possible to its further development. The August 2011 version of CheSAR has greater functionality - including an eSDS appendix - and many bugs have been fixed.

Making changes in the composition of a substance to be registered implies that a dossier needs adaptations on many points and that exposure assessments may change completely. Substance identification discussions should start as early as possible and should preferably be agreed before anything else is started, even if time pressure increases.

In order to produce CSRs starting from the data in IUCLID5 using the ECHA plug-in tools, the relevant data in IUCLID5 should be entered

in the appropriate boxes. For this purpose, high quality IUCLID5 files are needed.

The data - in particular the type of PNECs and DNELs - should be agreed upon as changes will impact the output of the risk assessments. This requires contact between toxicologists and industrial and environmental exposure assessors in an early stage and close cooperation between industry and consultants.

Getting the uses of a substance into a workable and informative life cycle tree and definition of short titles cannot be done without involvement of representatives of the supply chain. Both the sales department and the technical support departments can be helpful here.

The share of 'simple' mono-constituent substances in our portfolio was low. Many substances were characterised as 'UVCBs' (substances of unknown or variable composition, complex reaction products or biological materials), multi-component, or recycled materials. Each substance requires its own considerations and a standard approach for the risk assessment cannot be applied.

We expect that discussions on some registered intermediates may lead to a change of their status. Establishing an acceptable set of strictly controlled conditions may be of help here.

Another challenge is the timing of REACH. Before 2018 all substances need to be registered. However, many of the senior experts involved in the development of REACH will retire in this period, leaving a gap to be filled. Active knowledge management seems pivotal.

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