

RISK ASSESSMENT OF CHEMICAL CATEGORIES: CHALLENGES, LEARNINGS, PROGRESS OF ALCOHOL-BASED SURFACTANTS

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ABSTRACT

Several [voluntary] initiatives are ongoing simultaneously with the aim of assessing the health and environmental hazards and risks associated with the use of chemicals. By establishing the ERASM and HERA programmes and by participating in national and international HPV initiatives the Industry has demonstrated its capability to fulfil the significant requirements for a voluntarily risk assessment of several complex categories of aliphatic alcohols and their major surfactants derivatives. The methodology used in these programmes is flexible and applicable to single substances, complex mixtures and chemical categories; it is compatible with existing methodologies. A flexible approach to information collection and exchange between suppliers and formulators has been developed.

Working within a consortium is the way of the future. The New Chemical Policy in Europe (REACH) will require close collaboration and extensive exchange of information within value chains.

CHEMICAL MANAGEMENT PROGRAMMES FOR CHEMICALS

Over the last two decades, growing concerns have been expressed about a large number of chemicals being used to sustain the modern way of life. To address these concerns NGO's, national and international governments and Industry have started a variety of initiatives to evaluate the chemicals of concern. Initially, these programmes proceeded very slowly and prompted even further uncertainty about the safety of chemicals. For this reason a number of Initiatives were started in the late 1990s to address these concerns and to evaluate High Production Volume Chemicals within a five-year period. Examples of such data inventory and testing programmes are the US High Production Volume Chemicals Challenge Programme, developed in response to a challenge from the Environmental Defence Fund and the International Council of Chemical Associations (ICCA). This is the HPV Initiative. Other programmes were set up with the aim of addressing the safety of chemicals associated with specific uses or applications; an example of such an initiative is the Human and Environmental Risk Assessment on ingredients of household cleaning agents (HERA).

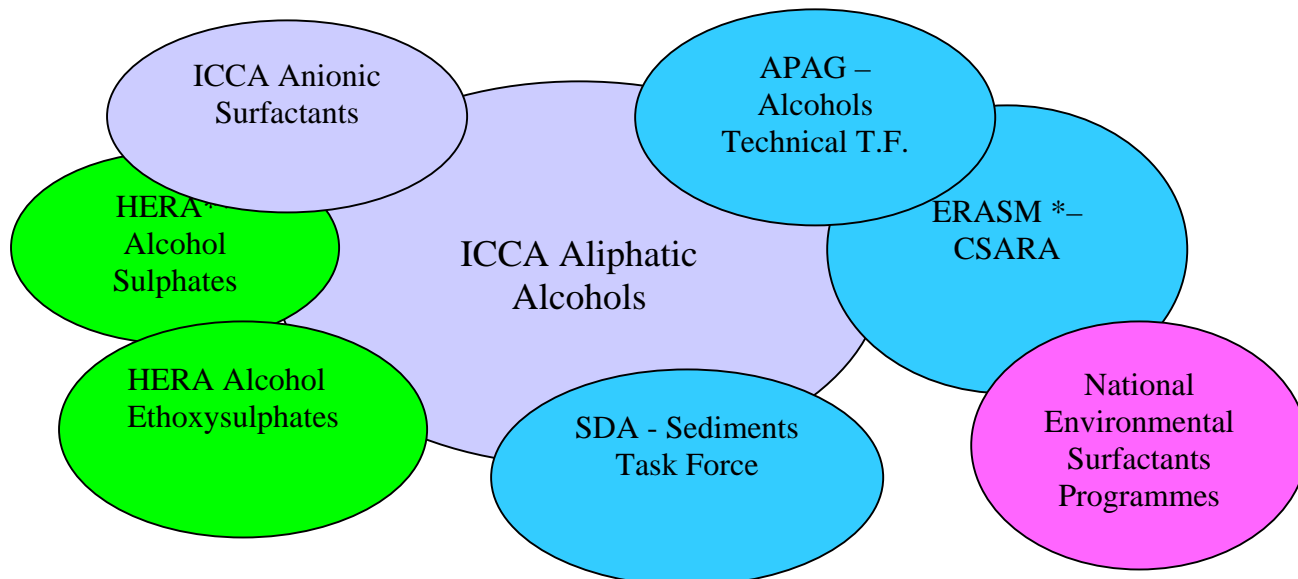
The Chemical Industry has taken up several of these programmes as a voluntary activity, but in some instances regulatory activity can be expected if the Industry activity fails to deliver.

Examples of Initiatives for Chemicals Management

- A. Initiatives on High Production Volume (HPV) Chemicals (Hazard inventory and testing of chemicals):
- OECD SIDS Programme (<http://www.oecd.org>)
 - Germany: Existing chemicals programme (Beratergremium für Umweltrelevante Altstoffe (BUA) (<http://www.gdch.de/taetigkeiten/bua.htm>)
 - US: EPA Challenge program (<http://www.epa.gov/chemrtk/>)
 - ICCA: Voluntary Global HPV initiative (<http://www.iccahpv.com>)
- B. Programmes for risk assessment of chemicals
- EU Risk Assessment of Existing Chemicals (<http://ecb.jrc.it>)
 - HERA Initiative (<http://heraproject.com>)
 - Concawe Risk Assessment of Oil Products (<http://www.concawe.be>)
 - 'Children's Health Initiative' (VCCEP) (<http://www.epa.gov/chemrtk/vccep/>)

CHEMICAL MANAGEMENT PROGRAMMES FOR ALIPHATIC ALCOHOLS & DERIVED SURFACTANTS

Many Aliphatic Alcohols and Anionic Surfactants are High Production Volume chemicals and therefore included as categories in the ongoing ICCA HPV Initiative. In addition, there are several other regional activities with International participation under the auspices of CESIO, APAG, AISE or SDA. A schematic overview of some key activities and links are shown below:



*ERASM, Environmental Risk Assessment and Management, created in 1991, is a joint platform of the European detergent and surfactants producers represented by their associations AISE (Association Internationale de la Savonnerie, de la Détergence et des Produits d'Entretien) and CESIO (Comité Européen des Agents Surface et de leurs Intermédiaires Organiques).

**The HERA project is a joint CEFIC and AISE project to assess the risk of the ingredients used in household cleaning agents for human health and the environment.

Overview of key internationally aligned programmes for aliphatic alcohols and surfactants.

Activity/Category	Output	Status: Q2 2004
Category Aliphatic Alcohols Programme: ICCA HPV: Aliphatic alcohols consortium Managed by: SDA	Output: SIAR Family: C6-C22 linear and essentially linear alcohols Conclusion: In progress	Draft SIAR under discussion Sponsor Country: UK
Category Alcohols Sulphates Programme: Human and environmental risk assessment Managed by: HERA	Output: Targeted Risk Assessment of AS used in house hold cleaning products Family: C12-C18 alcohol sulphates based on linear and essentially linear alcohol feed stocks Conclusion: No significant health and environmental risks	'Evergreen' draft published on HERA website, March 2002
Category Alcohols Sulphates Programme: ICCA HPV: Anionic surfactants consortium Managed by: SDA	Output: SIAR Family: C8-C18 alcohol sulphates based on linear and essentially linear alcohols feed stocks (includes AOS) Conclusion: In progress	Draft SIAR in preparation Sponsor Country: Germany
Category Alcohol Ethoxy Sulphates Programme: Human and environmental risk assessment Managed by: HERA	Output: Targeted Risk Assessment of AES used in house hold cleaning products Family: C12-C18 (EO 0-8) alcohol ethoxy sulphates based on linear and essentially linear alcohols feed stocks Conclusion: In progress; no significant health risks	'Evergreen' draft published on HERA website, Q2, 2004
Category Alcohol Ethoxylates Programme: CSARA Managed by: ERASM	Output: Monitoring based aquatic risk assessment of alcohol ethoxylates Family: C12-C18 (EO 0-18) alcohol ethoxylates based on linear and essentially linear alcohols feed stocks Conclusion: In progress	To be published in 2005

Initially, a strictly regional (EU, USA) approach was adopted to address the needs of the HPV and HERA activities, however it became rapidly clear that in isolation there was a significant duplication of effort and a lack of consistency between the regional databases. Differences in the scope or composition of the category are likely and inconsistencies in the evaluation or interpretation of the information might occur when conducted in isolation. These programmes require a significant effort, especially for the coordinating organisation, the lead company and the contractor collating and reviewing the shared - often confidential - information. By combining and aligning these efforts, a considerable saving of costs and resources can be achieved. The evolution of the approach adopted for the category of anionic surfactants is depicted below:

2000:	1. SDA signs up to US HPV initiative. Start of collation of hazard data; start of review activities 2. HERA initiates review of alkyl sulphates
	<u>Issues:</u> Incomplete (regional) collection of hazard data Inconsistent family description
2001:	Alignment of efforts: SDA coordinates activities; P&G/Shell Chemicals lead companies: Common hazard data base, consistent category, single contractor
2002:	HERA Risk Assessment published on HERA website
2003:	SDA signs up to ICCA programme. Germany lead country; Cognis lead company.

MANAGEMENT AND ORGANISATION OF COLLABORATIVE INDUSTRY INITIATIVES

Programmes such as the HERA and HPV initiatives require input from most of the participants and there is a need for leadership and coordination of the activities. Most of the activities are managed successfully through a single focal point. Associations such as CESIO, APAG, AISE, SDA all play a key role in managing on-going international cooperative programmes involving both manufacturers and the downstream Industry. These associations act as the secretariat for the Consortium and fulfil a key role as the clearing house for the large amounts of information collected by consortium members, provide the contractual and financial arrangements for contractors, and coordinate the communication with the membership, regulatory authorities and 3rd parties. In addition to the coordinating activities of the Industry Association, there is also need for technical leadership within the consortium. In most cases the Consortium identifies a 'lead company' to take on a leadership role within its membership. Experience has shown that alignment of the regional activities is best achieved through a lead company with a global perspective. Involvement of technical experts is also necessary from the start of the activities to ensure that all aspects necessary for a risk assessment are addressed adequately.

DATA REQUIREMENTS AND APPROACHES FOR THE RISK ASSESSMENT OF COMPLEX MIXTURES

Most commercial aliphatic alcohols and their surfactants consist of mixtures of homologous alcohols. Depending on the source and origin - oleochemical or petrochemical - and the manufacturing process, aliphatic alcohols used in the manufacture of surfactants may contain even and/or odd carbon numbers with linear or branched chains. Some of the alcohols consist of a single alcohol component, while others contain a distribution of several aliphatic alcohols. In the case of the ethoxylates and ethoxysulphates, a further complication occurs due to the formation of distributions of ethoxylates for each of the component alcohols. For this reason, members of the category of the aliphatic alcohols and the corresponding surfactants are categorised as 'Complex Mixtures'.

The principles used for a risk assessment of a complex mixture are similar to that of a single component and consist of the determination of a risk quotient, in which the predicted exposure and the predicted concentration without concern for adverse effects are compared. For a complex mixture, the risk quotient for each of the components in the mixture is added. The approach for an assessment of the human health risk deviates from the environmental procedure. In this case, the lowest threshold for a toxic effect (NOAEL) within the category is used for the risk assessment; it is also assumed that

human exposure consists exclusively of the mixture with the highest hazard potential, irrespective of the use of other products.

The standard information requirements for a risk assessment of a category of complex substances for the environment and human health are listed below. Although the information requirements for the assessment of a complex mixture are similar to those of a single substance, detailed knowledge of the composition of the 'complex mixture' is essential to enable an assessment. It should be recognised that several of the required parameters listed below can be estimated or calculated using mathematical models or QSAR's. The information requirements are:

1. General Information:

- Physical-Chemistry data:
 - Aggregation,
 - Water solubility,
 - Vapour pressure,
 - Kow
- Detailed chemical characterisation:
 - Carbon chain length distribution of each component
 - Linearity and characterisation of the side chain
 - Fraction of unreacted alcohols present
 - Degree/distribution of ethoxylation (AES)

2. Environment:

- Production volume total and breakdown for relevant use-categories
- Hazard data: for each of the components
 - Aquatic toxicity
 - Degradation

3. Human Health: (For mixture)

- Formulation data
- Use pattern
- Hazard data
 - Acute toxicity
 - Irritation and sensitisation
 - Repeated dose toxicity, including reproduction and development, carcinogenicity
 - Mutagenicity
 - Metabolism

For a category consisting of complex mixtures, the amount of information to be assessed is staggering. As an example, the category of the aliphatic alcohols consists of ca. 14 single component alcohols and more than 30 alcohol streams, representing most of the linear alcohols between C₆ and C₂₂ and 2-alkyl-branched alcohol between C₆ and C₁₆. The total number of entries in the IUCLID file (and Robust Study Summaries) for the phys-chem, ecotoxicology and toxicology chapters is more than 500 and excludes the compositional information.

DATA COLLECTION AND DOCUMENTATION

As discussed above, the quantity of information on the potential health and environmental effects for complex categories such as the alcohol and corresponding surfactants is enormous. The collection and selection of the hazard and exposure data are the most critical and time consuming steps in the development of a risk assessment. The success of this activity depends strongly on the cooperation of the suppliers and their customers to identify, collect and submit all relevant (eco)-toxicological information. Experience of current consortia has shown:

1. The literature search for well-established categories will result in thousands of hits requiring a significant input by the experts to screen and identify the information of relevance to the programme.
2. The standards adopted for the data reviews in the current programmes are higher than in previous activities. For this reason, the original data cited in existing reviews and publications

needs to be collected and summarised again; reliance on secondary information is no longer acceptable.

3. Identification of confidential information in company files is essential. A comprehensive data call-in is required in order to minimise potential for data gaps and avoidance of unnecessary testing.
4. The identification and collation of the key hazard, exposure and compositional data is labour intensive, very time consuming and requires input from experts.

In addition to the collation of the hazard data set, it is necessary to take account of the compositional information, production volumes and use categories. The members of the Consortium are requested to submit information on the composition and production volumes for different use categories to the Trade Association. This information is anonymised and aggregated by the Trade Association or a 3rd party contractor. Experience has shown that collection of such data is difficult and the information on the composition is often inconsistent between the consortium members. Similarly, production volumes for the different use categories are often incompatible with information from other sources. Although the process has been improved by using a standard format for these submissions, successful aggregation of the data is usually only achieved after a refinement of the submissions provided by the Manufacturer or the Formulator.

The draft exposure and hazard summary documents are prepared by ecotoxicology and toxicology experts from the lead company [or companies] or a 3rd party contractor. Clear guidance exists for the preparation of the documentation required for the HERA, OECD or EPA programmes and many of the technical experts are experienced in addressing the requirements.

LEARNINGS FROM THE ON-GOING INITIATIVES

The development of a voluntary risk assessment for complex categories such as the alcohol-based surfactants is very complex and involves many parties. The initiatives such as HERA and the ICCA HPV can only succeed if there is a close collaboration between all parties involved. It requires a strong leadership from the lead company and active support from the Trade Association. Direct involvement of business management is essential to ensure adequate motivation, resources and speed of the process.

The information gathering is the most critical phase of the process and often the rate-limiting step. Even highly motivated and active Consortia need considerable time to complete the data identification and gathering. Discrepancies in the information provided by the member companies are frequently observed and refinements of the information are needed to achieve the optimal consistency between the submissions. The uniformity of the data submission can be optimised if standard procedures, forms, templates are used, but even under optimal circumstances inconsistencies should be expected. Even for active consortia, the process of information gathering may well take up to 12 months from start to finish. Technical experts should be involved from the start of the programme to ensure that information obtained is adequate and meets the requirements

An on-going challenge for Industry sector initiatives is that companies providing a leadership role and dedicating significant resources to these activities appear to reap minimal commercial rewards for their extensive efforts made on behalf of the whole sector. Efforts invested by the Industry sector into the past and current Chemicals Management Initiatives are considerable, however in future such programmes will only succeed if **all** companies within the Sector participate and continue to share costs, information, data and resources.

These programmes have enhanced the reputation of the sector as a whole, but other direct benefits from participation in voluntary initiatives such as HERA and ICCA-HPV are uncertain and difficult to determine. It is therefore important to address the questions: 'How do we ensure that Industry efforts for programmes such as HERA continue and that leading companies are recognised for their contributions? Should customers make participation and/or compliance criteria for success in gaining its business?'

The cost of these initiatives is shared among the membership of the Consortia. The formula for cost sharing applied in the aliphatic alcohol and surfactant consortia consists either of an equal contribution from each of its members or a distribution of cost taking into account production volumes.

These approaches have proven to be an effective way for sharing of data/information and for development of risk assessments. The size of the membership of these consortia is sufficiently large that the outcome provides value for money and few problems have arisen with sharing of information and data for these activities.

Initiatives such as HERA, ERASM and the ICCA HPV programme have facilitated the development and validation of risk assessment methodologies for complex mixtures. Contrary to the standard regulatory approaches, the environmental models used in these programmes have the necessary flexibility to address issues associated with complex categories. Knowledge of a wide range of regulatory activities is required to identify opportunities for alignment, collaboration and consistency

ACHIEVEMENTS

By establishing the ERASM and HERA programmes and by participating in national and international HPV initiatives, the Industry has demonstrated its capability to fulfil the significant requirements for a voluntarily risk assessment of several complex categories of aliphatic alcohols and their major surfactants derivatives. The methodology used in these programmes is flexible and applicable to single substances, complex mixtures and chemical categories; it is compatible with existing methodologies. A flexible approach to information collection and exchange between suppliers and formulators has been developed.

ERASM and HERA are regarded as highly successful initiatives by external scientists involved in chemical risk assessment activities. All categories of the aliphatic alcohols and their major surfactants are being addressed in internationally aligned programmes.

Working within a consortium is the way of the future. The New Chemical Policy in Europe (REACH) will require close collaboration and extensive exchange of information within value chains.