Human & Environmental Risk Assessment on Ingredients of European Household Cleaning Products

Guidance Document Methodology

22 April, 2002

SUMMARY

HERA (Human & Environmental Risk Assessment) is a joint A.I.S.E.[1] and CEFIC[2] project initiated in September 1999. It concerns the assessment of the risks to human health and the environment from ingredients of household cleaning products during the two scenarios 'Use in the Household' and 'Disposal to the Environment'. It is not concerned with later aspects in the risk assessment process such as risk reduction, although its output is likely to be of great value in managing any risks identified.

HERA is a two-phase project and is managed and run by a team of task forces and other fora specialising in the provision of resources, expertise in risk assessment and in communication. A web-site has been developed and databases are being populated with the necessary data on intrinsic properties, exposure and use of each HERA Substance. Workshops with stakeholders are being planned.

The first phase of HERA has the aim of preparing and testing a robust risk assessment methodology. The second phase will utilise the methodology to assess all of the important ingredients to be found in household cleaning products marketed by A.I.S.E. companies.

This document details the procedure for performing the risk assessments.

[1] Association Internationale de la Savonnerie, de la Détergence et des Produits d'Éntretien (International Association for Soaps, Detergents & Maintenance Products)
[2] European Chemical Industry Council

FINDING YOUR WAY THROUGH THIS DOCUMENT

This document is a manual for risk assessments using the HERA (Human & Environmental Risk Assessment) methodology

The Guidance Document begins with a general section (1.1-1.9) which introduces the concept of HERA targets (1.1), both in terms of chemicals (1.2) and use scenarios (1.3). The generic principles of the HERA risk assessment process are outlined in 1.4. Sources of data are discussed in 1.5 and a first indication of the HERA report structure is given in 1.6, although the detail for this subject has been consigned to Appendix B. The roles of members of the HERA Team are summarised in 1.7. The results of the risk assessment will be communicated (1.8) and a database has been created (1.9) for the storage and retrieval of both data and the basis of each decision made by the Task Forces and Substance Teams.

Section 2 concerns environmental risk assessment in HERA. The focus on certain aspects of the environment is treated in 2.1 to 2.3; this represents an important series of decisions for HERA. Figure 2 demonstrates the whole environmental process and can also be used as a guide to the reader. The environmental effects aspects are introduced in 2.4, including data quality criteria, and the exposure and effects calculations using a modified form of the EUSES program are described in 2.5. For the environment there is a specific exposure scenario for detergents (2.6) and refinements of this are explained. Inorganic and other naturally occurring substances need to be considered and these are discussed in 2.7. The environmental scientists must also have in mind the possibility of risk to humans *via* secondary or indirect poisoning, as outlined in 2.8. Finally a section (2.9) is presented on confidence in the adequacy of the assessments, with notes on uncertainty analysis and relevance.

Section 3 covers the human health assessment procedure. The scope is defined in 3.1 and the process is briefly described in 3.2 and in Figure 5. The exposure of consumers in the home is explained in 3.4 (and in Appendix D) and hazard data (collection, validation etc) in 3.5. An output of the human health assessment is the 'Margin of Exposure' (3.6), and the important stage of characterising and drawing conclusions from the assessment is given in 3.7.

The document has five appendices describing the data requirements, report structure, data quality, consumer exposure models and a spreadsheet for the input of HERA data for the purposes of the EUSES program.

METHODOLOGY OF RISK ASSESSMENT IN HERA

SECTION 1 – GENERAL INTRODUCTION TO HERA RISK ASSESSMENT

The HERA risk assessment methodology uses a focused and tiered approach to both hazard and exposure assessment. It also includes certain restrictions in the selection of substances and the scope of the overall risk assessment.

This section covers the areas common to both human health and environmental risk assessments. The organisation of HERA is summarised in Figure 1. The organisation is designed to ensure full communication and collaboration among the members of the HERA Team. The roles of each sub-team within the HERA organisation are given in section 1.7.

1.1 HERA focus

HERA focuses on

- chemical substances used primarily in household detergent and cleaning products marketed by A.I.S.E. member companies;
- consumer use of such products (*i.e.* not professional or workplace use); including intended use, but also, for the human health assessment, other foreseeable uses and accidental uses;
- endpoints of concern for consumer exposures expected from A.I.S.E. member company products;
- environmental compartments of relevance.

HERA operates 'downstream' of the manufacturing and distribution processes (Figure 1) – aiming to assess risk and thus afford protection in homes and in those environmental compartments (eg sewage treatment plants, rivers, farmland and potentially the sea) which may receive the remains of the ingredients and their breakdown products. The human health assessment considers all reasonable and some possible but abnormal exposure to the substances in the domestic situation. The environmental assessment principally evaluates the use and disposal phase of substances, as this is the major route by which household detergent and cleaning products can enter the environment.

Excluded scenarios

HERA deliberately does not address human safety during the pre-use stages of the life of the chemical. Neither are industrial and institutional (I&I) uses of the same chemicals included, nor spills or other accidental releases. The assumption is made that supplier companies will have sufficient safeguards and controls already in place for their workers and the environment to cover the manufacturing and distribution stages of HERA substances. Also, control systems for professional use will be defined and maintained by the I&I users, and environmental releases will be localised and minimised as part of good manufacturing practice. Similarly the formulators

have such systems in place in and around the factories where the ingredients are used to manufacture the formulated cleaning products and during distribution through the retail trade. On the other hand the domestic post-manufacture stages are outside the control of the supplier and formulator but have been considered to require the responsible approach exemplified in HERA.

Figure 1 **The scope HERA assessments**

Area for attention	**manufacture of ingredient**	**formulation of product**	**use of product**	**treatment & disposal of product**
Human health	occupational regulations		household	food chain
Local environment	agreed locally		yes	yes
Regional environment	effectively within HERA		yes	yes

In the figure, the lightly shaded area shows where HERA applies. The HERA methodology also gives regional environmental releases which include the contributions due to production and formulation. Further information can be found in Chapter 2.5.1.

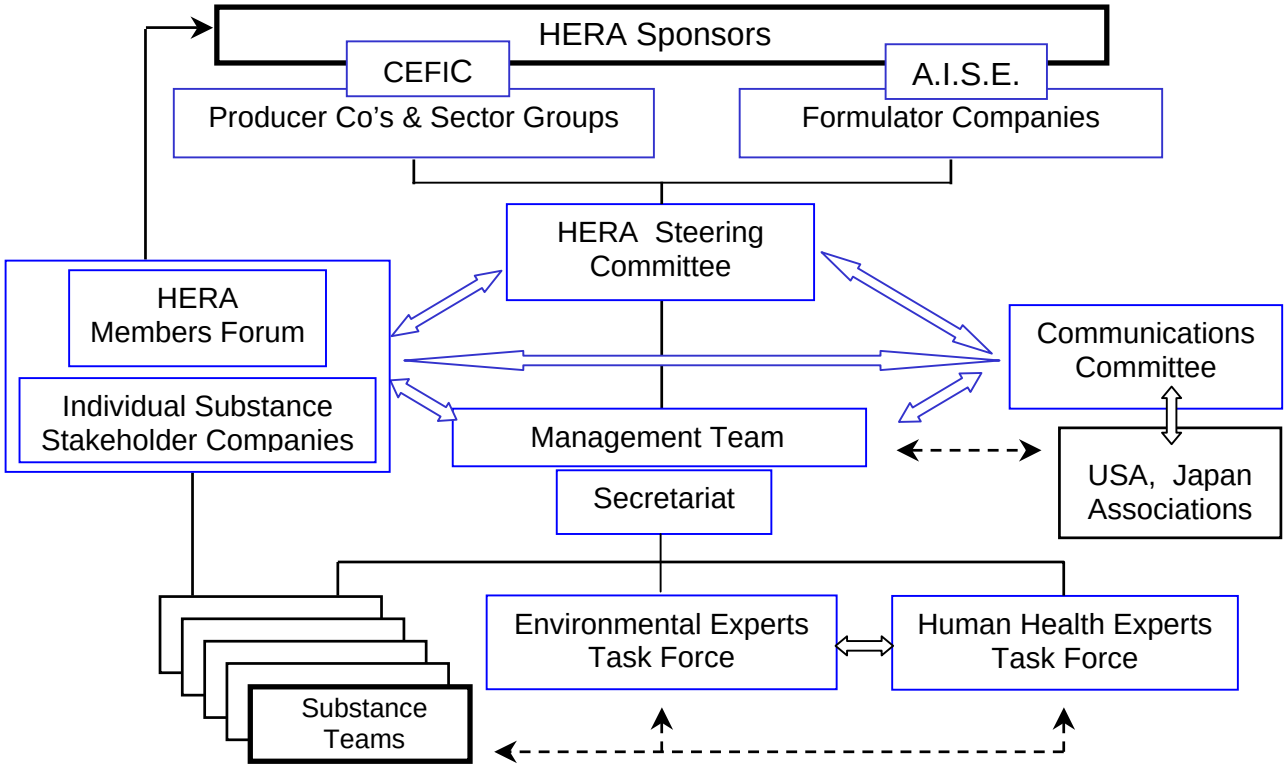


Figure 1 The organisational structure of HERA

1.2 Selection of Chemical Substances

HERA focuses on chemical substances[3] used primarily as ingredients for household detergent and cleaning products. The range of household products includes fabric washing products (*i.e*. fabric washing powders, liquids, gels and tablets), fabric softening products, hand / machine dishwashing products and general hard-surface cleaning products, such as bathroom or kitchen cleaners. For the human health assessment, ingredients used solely in consumer products such as personal care products (*e.g.* shampoo or toothpaste), or cleaning products intended for institutional and professional use, as well as workplace exposure, are not included. However, for the environment, not withstanding HERA's focus on household detergent and cleaning products, the HERA initial assessment uses total annual production volume and therefore in the lowest tier of HERA other significant uses are also included.

1.3 Selection of Use Scenarios

Consumers
HERA will evaluate the risk posed to the consumer from exposure to the chemical substance during intended use and foreseeable uses of A.I.S.E. products. Accidental exposures are included in the human health scenarios where relevant.

[3] See glossary for the definition of "substance" as used in the context of this document; substances sometimes are also referred to as chemical substances, ingredients or raw materials.

Environment
HERA will evaluate the risk posed to relevant environmental compartments from exposures and releases during or after product use by the consumer, as this is the primary means by which household detergent and cleaning products can enter the environment.

1.4 The Risk Assessment Process

The following procedure for focused risk assessments of chemicals has been adopted, based on the tiered approach for conducting risk assessments currently accepted within international bodies such as OECD and the European Union. These procedures are described in more detail for the environment (Section 2) and human health (Section 3).

1.4.1 Substance characterisation

For each chemical chosen for risk assessment, the HERA methodology must:

- identify the substances (possibly with different technical specifications) used in different types of A.I.S.E. products, with associated CAS numbers if possible;
- describe the composition of the substance, including the homologue characterisation and distribution - and any impurities;
- where needed, identify data from related substances (*i.e.* same or closely related chemical substance, but different Chemical Abstracts (CAS) number), if data for the commercially used substances are not available.

CAS numbers
Often ingredients in detergent and cleaning formulations are made on a large scale by a number of producers. Although nominally the same, competing and interchangeable materials often have minor differences in their chemical structures with little effect on performance. Thus several CAS numbers may be in use for what is nominally one material. In addition, one class of chemical may be produced in many closely related grades, tailored to provide formulation, handling and performance variations. Most of the surfactants fall into this category. If justifiable, it is desirable to group these related substances and evaluate them in one risk assessment.

Each risk assessment should contain a list of substances and their CAS numbers considered, and should document their use in the risk assessment.

1.4.2 Group formation for household detergent and cleaning product ingredients

Justification can be made for grouping a series of like chemicals when their physico-chemical and toxicological properties are similar or follow a regular pattern as a result of structural similarity. Criteria for category formation for the HERA initiative are chosen by analogy to the rules described for the OECD SIDS programme which is the basis for the ICCA HPV initiative (Guidance for the Development and Use of Chemical Categories in the HPV Chemicals Program, http://www.oecd.org/ehs/hpv.htm). Equally, it may be important to justify why a grouping cannot be used: this may be the case if a proposed grouping includes several different modes of toxic action.

There are two scenarios under which it may be beneficial to consider collectively groups of molecules in HERA risk assessments:

- Many household detergent and cleaning product ingredients, especially surfactants, are complex substances. The components of such substances are usually structurally related giving rise to predictable patterns of fate and toxicity. This may be considered as **"within substance grouping"**.
- Some household detergent and cleaning product ingredients are similar to others in terms of their structure and chemistry, although they may have different CAS numbers. This may be considered as **"between substance grouping"**.

In both cases potential benefits of grouping are a reduction in the complexity of the assessment, while at the same time increasing its realism and comprehensibility.

Typically, 'groups' should consist of molecules whose physico-chemical and ecological, or toxicological properties are expected to be either similar, or to follow a regular pattern as a result of high degree of structural similarities. Examples for several substances are given in the OECD ICCA HPV guidance. Both "within substance" and "between substance" grouping can be applied to surfactants and to other selected HERA substances. For example, each alkyl sulphate substance is composed of a homologous series of molecules that differ in carbon chain length and degree of branching. Test data are available for some of the individual homologues, but not for others. By grouping the components of an alkyl sulphate substance a better understanding of the fate and effects of the substance will be gained. Similarly, there is a family of alkyl sulphate substances, each with a different homologue distribution. By grouping the family of substances the fate and effects of these related chemicals can be investigated more efficiently.

Groups can be constructed based on structural similarities such as common functional groups, or on considerations of chemical or metabolic equivalence. A description should be given of the grouping criteria such as general molecular structure, carbon chain length and degree of branching, etc. Furthermore a list of all substances (*i.e*. individual CAS numbers) or components covered by the group should be provided. The following criteria can be used as the basis to establish chemical groups:

1. **Structural Similarity** Chemicals that form a homologous series or that are structurally similar may be grouped together. A homologous series is defined as a series of molecules in which each member differs from the next member by a constant chemical unit (*e.g.* alkyl chain length, number of ethoxylate groups, number of chlorine atoms, etc.).

2. **Route of Exposure** Structurally similar molecules may or may not demonstrate consistent trends in properties, and thus may have to be subdivided into groups with a common route and level of exposure. These groups should be based on the physical/chemical properties (*e.g.* vapour pressure, water solubility, or K_{ow}) that determine, for example, the partitioning of a material group in the environment.

3. **Mechanism of Toxicity** Only structurally similar molecules which have a common mode of action can be grouped together.

To run separate focused and isolated environmental or human health risk assessments for each individual component of a complex substance would be unnecessarily burdensome and confusing: transparency would be lost due to the

great number of risk assessments of comparable components. Thus similar components should be grouped when this can simplify the risk assessment process.

In the HERA environmental risk assessment, for those detergent ingredients where grouping can be justified, the "additivity" mixture toxicity approach (which is implemented in EUSES as the hydrocarbon block method) can be applied. This method assumes additive toxicity for a mixture of closely related molecules found in the environment. In practice, the overall PEC/PNEC of a chemical category is calculated as the sum of the individual components' PEC/PNEC ratios. This way, the overall risk assessment of a chemical class can be based on its (expected) environmental fingerprint. Since additivity of toxicity is likely within groups which are structurally related, this approach is more realistic than assessing individual components separately.

Grouping can also be useful as part of a programme to fill data sets, as described in the OECD ICCA HPV guidance. Often, data are available for only the key commercial distributions or for a number of individual components of a group - but not for all individual components nor all commercial products. For example, for a given surfactant, data from a higher tier study such as a mesocosm or chronic / subchronic study may exist for some homologue(s), whereas limited acute data may be available for other homologue(s). Within a group, it is possible to predict the properties of data-poor components by interpolating between data-rich components. To justify this, the relationship between the structure and the activity (*e.g.* toxicity, adsorption) in the category must be sufficiently well understood to enable prediction of untested endpoints for single members of the category, ideally by interpolation or justified QSAR assessments.

If molecules are grouped into categories in a HERA environmental or human health risk assessment, the specific risk assessment should contain the justification of the grouping procedure used. Any "between substance" grouping should be common to both the human health and the environmental risk assessment. It is noted that due to differences in exposure pathways, or for reasons of data availability, it may be necessary for the HERA environmental and human health risk assessments to form different "within substance" groups. However, common grouping procedures will be encouraged.

If a class of analogous chemicals is evaluated as a single group in the HERA Risk Assessment process, the HERA Report should present:

- description of chemical class/category;
- identification, composition and relevant properties of individual members of the class;
- justification for grouping of chemicals within a category.

1.4.3 Assembly of data

Assemble physico-chemical, toxicological and ecotoxicological data on the chemicals concerned from databases *e.g.* IUCLID, BUA, IPCS and other published data compilations and the internal databases of company members (see also *Data sources 1.5)*. An overview of potentially useful data for consideration is given in Appendix A.

General
As well as the data particular to environmental or human health risk assessments (see below) the HERA risk assessment reports will take into account the following general points:

- results of validation for data quality, robustness and GLP;
- justification for read-across, route and species inter/extrapolation and (Q)SAR and consideration of data gaps;
- derivation of the PNEC, or the NOAEL or threshold for each of the critical endpoints.

1.4.4 Information on the use/s of the substance

The use levels of individual chemicals in the various relevant classes of household detergent and cleaning products, *e.g.* laundry detergents, household cleaners, fabric softeners etc must be established and included in each HERA report.

1.4.5 Tonnages

The tonnages of each chemical released following use will be determined, and the source of the tonnage information will be clearly stated in each HERA report. Tonnage information may be obtained from producers, and may include import and export information. Complementary information from the formulators of detergent products about the tonnage released from detergent use may also be provided. This will be used to predict exposure in environmental compartments, *i.e.* soil, air, water and sediment as relevant to derive the Predicted Environmental Concentration (PEC). If available, appropriate monitoring data will be included.

1.4.6 Human exposure

Human exposure is to be defined through consideration of intended use, foreseeable uses or accidents for each class of products.

The section on human exposure will present for each ingredient under consideration an overview of the habit and use pattern and its maximum concentration in different product types. On this basis the relevant routes of consumer exposure will be determined and the calculation of the direct exposure to consumers for each exposure scenario using the relevant consumer exposure models will be presented in the HERA report. Also, the total direct dose will be estimated. Exposure *via* the environment and/or other sources will be included in the calculation of the overall dose.

The report will highlight :

- identification of all direct and indirect human contact sources;
- justification of exposure routes selected for further assessment for the consumer;
- justification of the model parameters used in the different exposure scenarios;
- assessment of potential exposure resulting from foreseeable and accidental uses.

1.4.7 Conduct of focused risk assessment

Environment
The environmental exposure and effects assessments will be combined to produce a risk quotient, or PEC/PNEC value. This will be documented in a risk assessment chapter, which will include a treatment of the uncertainties of the most sensitive parameters as part of a description of the overall confidence in the risk assessment

Human Health
For human health, the section on the risk assessment will present the margin of exposure (MOE), if appropriate, calculated for each of the critical endpoints. This section will address risks associated with the normal use patterns but may also address foreseeable and accidental uses. The Human Health risk assessment chapter will also include a treatment of the uncertainties in both the hazard and exposure assessments.

1.5 Data Sources

Hazard assessment should be based on toxicity data which have been evaluated with regard to reliability, adequacy, relevance and completeness. For many existing substances the test data available will have been generated prior to the establishment of standard protocols and GLP. To address the potential variability in data quality in older data collections, there are various possible approaches. It is proposed in HERA that the criteria as described by Klimisch *et al.* (1997) and OECD (2000), see Appendix C, should be used as the starting point for a "validity check".

The HERA environmental effects data quality criteria described in **2.4** develop the recommendations of Klimisch *et al.* (1997) and the TGD. In all cases, there is a need for a critical evaluation of effects data to confirm that these really reflect the intrinsic toxicity of the substance.

Further data on structurally similar substances may be available and these may add to the toxicity or ecotoxicity profile of the substance under investigation.

Risk assessment in the framework of HERA is based on data for substances and sometimes products from different sources, *e.g.* scientific literature, IUCLID and other published databases and company in-house data. In the case of human health risk assessment, 'observational' data on man from exposure to the substances or products containing those substances may be available *e.g.* data from epidemiological studies, Poison Control Centre studies, accident surveys and clinical reports and other records of consumer or worker experience. Further, human volunteer studies may also contribute additional complementary information to a risk assessment (Roggeband *et al.*, 1999).

Risk assessment is an iterative process. If significant data gaps are identified, then steps may need to be taken to obtain the missing values. Alternative strategies will depend on the particular substance. In some cases it may be appropriate to take risk reduction measures and in others it will be more appropriate to generate data to close the gap. If significant data gaps are still present, then the relevant HERA Task Force Chairman should be approached with a view to appealing to A.I.S.E./CEFIC member companies to see if they have any data not yet made available to HERA. If not, the HERA Management Team, Members Forum or Steering Committee may have to be approached to see if there is support to carry out the necessary tests.

1.6 HERA Risk Assessment Report Structure

For each of the HERA Risk Assessments a report will be produced. The reports will describe the hazards and exposure estimates of the major ingredients to the environment and the consumer through the use and disposal of household detergent

and cleaning products. Based on the hazard and exposure information, the HERA report will present an assessment of the risks for potential adverse effects to the environment and the consumer.

The format for the HERA risk assessment report should be similar to that of the OECD SIDS Initial Assessment Report (SIAR), with modifications as needed. Guidance for the preparation of OECD SIAR reports can be found at:

http://www.oecd.org//ehs/ehsmono/revisedsiar.doc

Appendix B shows the main headings of a typical report.

1.7 Roles

The following flowchart (Figure 2) should be regarded as a summary to assist the Substance Teams.

The chemical substance **raw material suppliers** will prepare a hazard assessment for both environment and human health effects. Where meaningful, collaboration of raw material suppliers within a consortium is possible. In addition, they will supply tonnage data, if necessary in confidence *via* a 'consortium administrator', targeted, if possible, to tonnages used in A.I.S.E. products. If resources within a company are limited, consultants could assist in this step.

The **product formulators** provide exposure assessments for the environment and human health, including data on the concentration ranges of the substances used per product category (e.g. hard-surface cleaners, fabric softeners etc) and information on total releases. These substance-specific data are forwarded from the formulators *via* A.I.S.E. if necessary in confidence, to the risk assessor.

The **risk assessor** will draft the HERA risk assessment report. The assessor may be a consultant, especially, if risk assessment resources in the company are limited.

The **HERA Task Forces** (Human Health and Environment) will peer review the draft report. The key producers and users of the particular chemical participating in HERA will review and release the report. When complete, the risk assessment is submitted to the **HERA Members Forum** and **Steering Committee** for, respectively, final comment and approval.

1.8 Communication of the risk assessment on a substance

It is intended to publish HERA risk assessment reports on the internet (after final approval by the HERA Steering Committee).

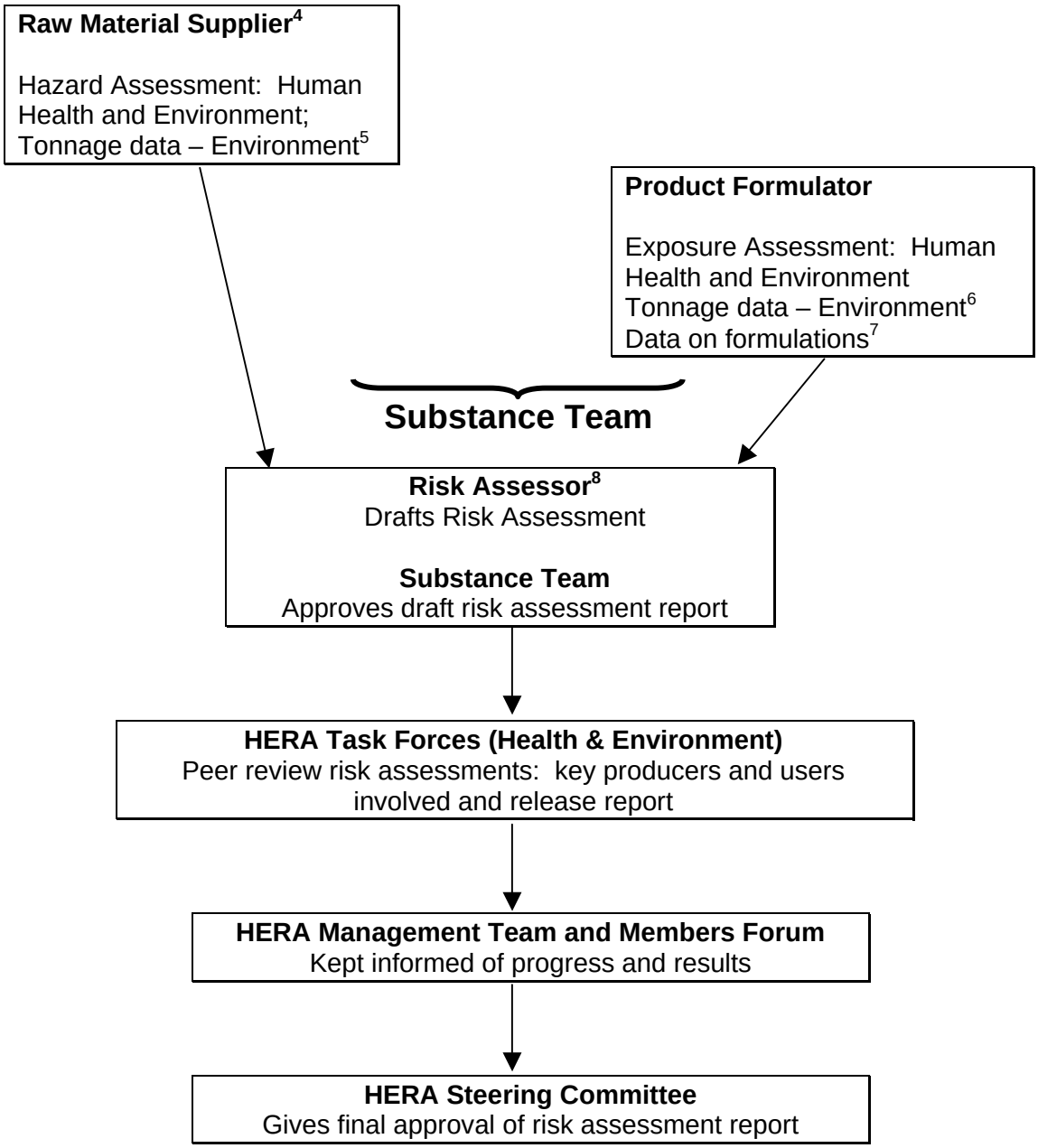


Figure 2 Generalised procedure of HERA

(Note the sequence of Raw Material Supplier involvement preceding Formulator involvement.)

[4] Possibly in collaboration within a supplier consortium: always in collaboration where there is more than one supplier.
[5] Confidential
[6] Confidential
[7] Confidential
[8] Can be a consultant and also operate as a trustee.

1.9 Storage and retrieval systems for data and decisions

Information collected during the HERA process will be centrally stored in an electronic database. This database will contain the following information:

- data that have been used for the HERA conclusion;
- justifications for data/endpoint inclusion / exclusion in the HERA assessment.

It is the intention to make this database publicly available and searchable through the internet in phase II of HERA.

SECTION 2 – GUIDANCE ON RISK ASSESSMENT FOR THE ENVIRONMENT

2.1 Scope of HERA Risk Assessment for the Environment

HERA provides a methodology for Environmental Risk Assessment which is focused on the ingredients in detergent and household cleaning products marketed by A.I.S.E. member companies. For the environment HERA focuses on the use phase of product ingredients, as disposal following use is the source of most of the total chemical tonnage which reaches the environment. Thus for the local scenario, environmental releases from either specific or generic local production and formulation sites are not included, as this is outside the scope of HERA. For the regional scenario, releases from production and formulation sites are incorporated into the overall releases to the region, as shown in Section 2.5.1.a.

2.2 The HERA Environmental Risk Assessment Process

As part of a focused environmental risk assessment, HERA uses the principles and tools described in the EU Technical Guidance Document (EU TGD, 1996). This begins with the use of the EUSES model, though default parameters are refined to make them more specific to detergent and household cleaning products. This is done as part of a tiered risk assessment process, reflecting a general principle of the risk assessment of chemicals and acknowledging that the process is data driven. In compliance with the EU TGD, the HERA risk assessment will not proceed beyond the point that shows safety according to generally applied criteria (PEC *v* PNEC). Hence, in the early stages of this process, selection of the most conservative data may lead to a risk assessment result which may suggest evaluation of higher tier data.

The environmental risk assessment is based on a detergent-relevant exposure assessment (PEC) (See 2.6) and an effects evaluation based on existing ecotoxicological data (PNEC). Further ecotoxicology endpoints not specified in the TGD may be included in the HERA environmental risk assessment for specific chemicals where these effects are thought to be potentially significant.

At present, the HERA environmental risk assessment methodology contains several distinct stages (Figure 2), which apply to each product ingredient chosen for evaluation. As specified in the TGD, degradation products or metabolites which are stable or toxic will be included in the HERA assessment. The process to be followed in the HERA assessment contains these essential steps:

- Select the chemicals for evaluation from those used in detergent and household cleaning products **(see section 1.2 for further information)**; the forming of appropriate groups of substances **(1.4.2)** should be considered as part of this process.
- Characterise the chemical selected, including the appropriate CAS numbers, and other necessary data such as hydrocarbon chain-length distribution for surfactants, and minor components present **(1.4.1)**, forming groups of components as necessary **(1.4.2)**;
- Assemble physico-chemical, ecotoxicity **(1.4.3)**, fate and environmental data on the chemicals concerned from databases *e.g.* IUCLID and other published data compilations or unpublished company members' databases **(1.5)**;

- Establish the tonnages of each chemical released to the environment **(2.3)**;
- Use the EUSES model including justified amended HERA default values to carry out the environmental risk assessment **(2.5)**, as part of a tiered risk assessment methodology .
- Determine the exposure of each of the environmental compartments *i.e.* soil, air, water, and sediment, using models and, if necessary, available monitoring data **(2.5 and 2.6)**;
- Evaluate the uncertainties involved in the focused risk assessment process **(2.9)**.

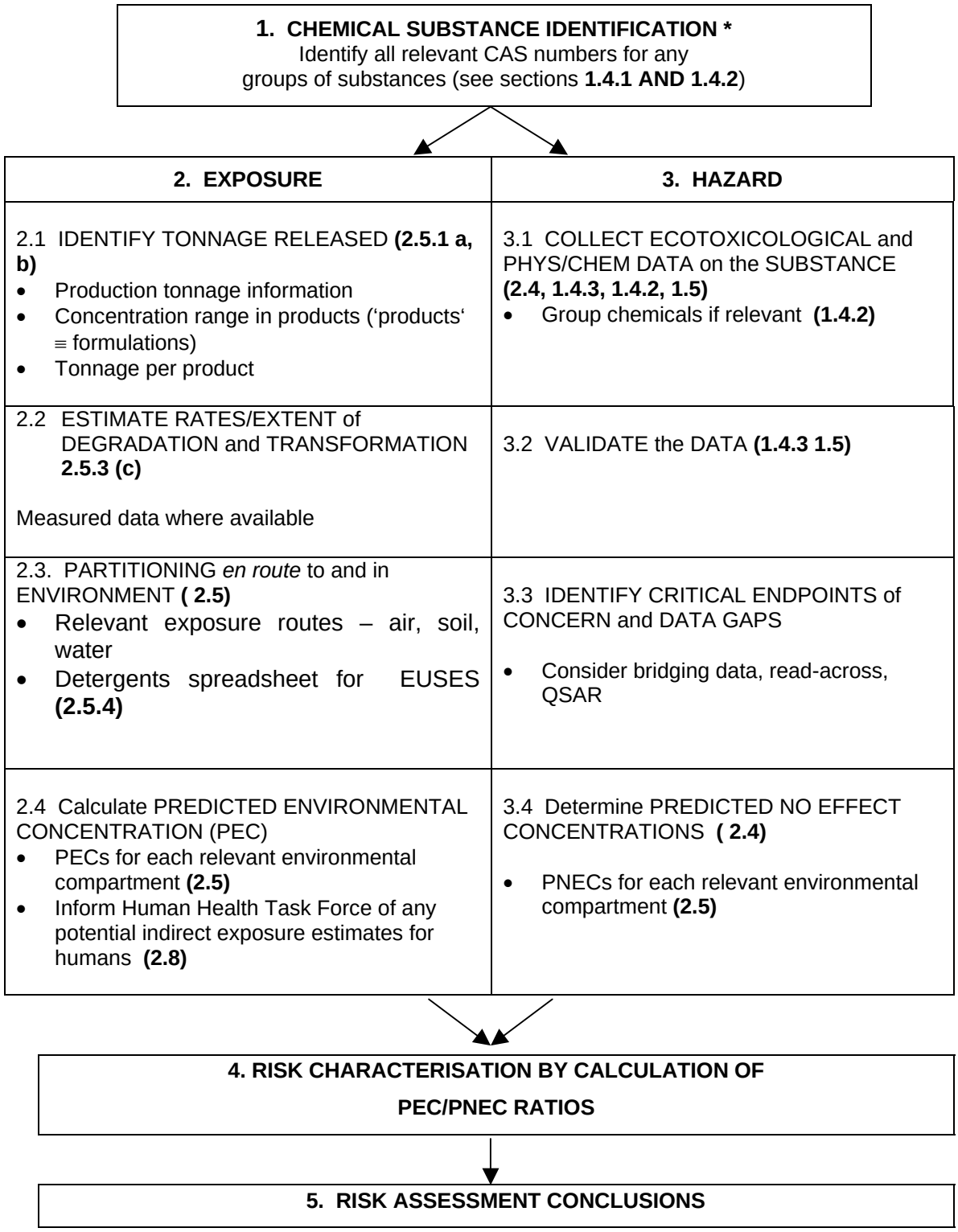
In addition, the document contains two special sub-sections on evaluating risks from inorganic substances **(2.7)** and on predicting the likelihood of indirect exposure to humans **(2.8)**.

2.3 Environmental Release of Substances

The first part of the HERA risk assessment process which is specific to the environmental risk assessment is the determination of the amount of the chemical which will be released to the environment. Estimating with precision the amount of a chemical substance used or released can be a surprisingly complex task due to competitive and confidentiality concerns within industry. Companies must also comply with national and European competition laws. Trade associations such as CEFIC have therefore developed strict rules for use in collecting and processing industry production and/or sales data (CEFIC, Ecostat Data Processing Centre, "Handling confidential statistics in compliance with competition laws", June 1997).

Two approaches may be used starting either from production or usage estimates. (1) According to the tiered approach which is followed in the HERA risk assessment, the total European production figure of the chemical will be the starting point for the exposure calculations but (2) this may be replaced or supplemented by tonnage data addressing more specifically the use in the detergent product categories.

(1) The first approach assumes that all of the material produced in Europe or placed on the market in Europe is used in Europe (or the region of interest for the risk assessment), and that all of this material is used in products marketed by A.I.S.E. member companies. This information must be obtained from the producers of the chemical substance. In many cases, good summary information will be available from a trade association. This method will give an over-estimate of the amount of the substance released, unless imports exceed exports plus other, non-A.I.S.E. uses. If information on export and import volumes and on non-A.I.S.E. uses is available, this should be included in the usage estimate. Note that the A.I.S.E. use pattern involves wide dispersive release – *i.e.* full release of the substance to the environment during use and disposal. This is the worst case, maximum release scenario. Local PECs for production and formulation are not specifically included here, because the TGD assumes that these account for approximately 1% of the total production tonnage (see section 2.5.1.a). More realistic release scenarios may involve a reduction in the fraction of total chemical released to the environment and will be used where appropriate, and will be justified on a substance-specific basis as part of the tiered risk assessment approach. Production and sales information will normally be



*This step is common to both the Human Health and Environment Methodologies.

Figure 2 Overall Environmental Risk Assessment Process

regarded as confidential by producers. Where detailed information is required, to preserve confidentiality it will often be necessary to provide a means to contribute data to an independent body such as a consultant or a trade association for compilation.

(2) The second method for determining the amount of a substance released to the environment requires knowledge of the amount of the chemical used in each product in which the chemical is used, and knowledge of the annual sales volume of each product. The information required will be at the brand, and possibly at the brand variant level. The sales volume information is often available from market research companies but is usually sold to commercial organisations such as the product formulators with the proviso that it should not be distributed to third parties. The sales volumes and formulations of the different brands and brand variants produced by the formulators are commercially confidential. However, it is possible for formulators belonging to a trade association such as A.I.S.E. to use the formulation data and sales volumes for their own brands to calculate the amount of the substance sold in their own products for a chosen year. The trade association then combines the amounts of the substance sold by each of the member companies to produce an annual sales volume for the substance. This will be an under-estimate of the actual amount of the chemical sold, unless all formulators participate in this trade association activity. Participating formulators may try to extrapolate their data to the rest of the market, by estimating the formulations and sales volumes of those formulators who do not participate in the trade association activity. Unpublished information from several European detergent formulators has been used to estimate the uncertainty in this process to be less than 10%. Thus this should not be a limiting factor in improving the uncertainty of the overall HERA environmental risk assessment process.

If the available data and the chemical use patterns allow both methods to be used, then convergence of the results of the two methods adds confidence in the reliability of the data, and an estimate of the associated uncertainty. Provision of both types of tonnage information is preferable. The individual HERA risk assessments must clearly state the source(s) of the tonnage information used.

2.4 Environmental Effects

The ecotoxicological effects assessment within HERA follows the tiered approach, as set out in the TGD. Hence, the HERA assessment will take the higher predictive value of long-term ecotoxicity data into account. If, for example, at least two subchronic/chronic data points from different trophic levels are available and these include the type of organism shown to be most sensitive in the acute studies, the acute toxicity data will not be considered further for the PNEC derivation.

Probabilistic treatment of chronic ecotoxicity data may be used at the highest tier of the risk assessment process, if enough information is available. Effects data from mesocosm studies are probably most useful for validation of the probabilistic or the deterministic approach. If any modifications to the TGD default assumptions are made, they must be fully explained and justified for each specific risk assessment.

In the HERA environmental risk assessment, QSARs can be used to derive 'toxicity scaling factors' between different homologues of a surfactant category (see

section 1.4.2) The ratio between the toxicity QSAR prediction for a data-rich and a data-poor homologue can then be used to extrapolate the data-rich homologue's effects data (or even PNEC) to the data-poor one. Within one group of chemicals, a similar approach can be used to re-scale different chronic toxicity data points from different homologues to a single (*i.e.* average) structure, hence leading to a large data-set for this structure, which may subsequently be used to derive a PNEC using the statistical extrapolation method.

2.4.1 Assessment of ecotoxicology data quality

The balance between the speed at which the HERA environmental risk assessment can be carried out and the requirement to take all the available hazard data into consideration and to document the decision process for using or rejecting them must be decided for each substance by the individual HERA substance teams. This will be a major determinant of the efficiency of the HERA risk assessment process. Other requirements to gather hazard data for a specific substance, for example, in support of the ICCA, OECD, or other voluntary initiatives, may influence the choice as to the most efficient way to balance the speed of the risk assessment and the reliability of the data used in the risk assessment process.

Although the lowest, *i.e.* the most sensitive effect concentration of each individual endpoint of the data base is the starting point of the HERA evaluation, the final decision on the data to be used for the PNEC derivation depends on the data quality and relevance. In all cases, there is a need for a critical evaluation of effects data to check whether these really reflect the intrinsic toxicity of a chemical or are more related to specific test conditions. In particular, data referring to sparingly soluble substances should receive appropriate scrutiny.

2.4.2 General guidance concerning the scientific criteria for data selection and evaluation

Selection of data for a HERA risk assessment is based on a set of quality criteria to indicate which data are preferred. If no data meet the quality criteria, the available data may still be accepted if it is evident that they are likely to be conservative. However, data that are in line with the quality criteria will automatically be preferred. The purpose of defining quality criteria is to encourage consistency and transparency between the HERA risk assessments. The HERA data quality criteria develop the recommendations of Klimisch *et al*. (1997) and the TGD (see Appendix C). Data of doubtful validity will be rejected, and will not be used in the HERA risk assessments.

2.5 Application of EUSES in the HERA Environmental Risk Assessment

The European Union System for the Evaluation of Substances (EUSES) has been chosen as the basic tool to perform the HERA environmental risk assessment calculations. All deviations from standard EUSES default values are justified here, or will be justified in the individual HERA risk assessment reports. EUSES is based on the recommendations of the EU Technical Guidance Documents (EU TGD, 1996). The HERA detergent scenario is described in section 2.6. Modifications to EUSES for exposure (2.5.1) which are used in the HERA approach, and the minimum data

requirements for the EUSES model (2.5.3) are given below. Note that the exposure assessment of the HERA environmental risk assessment process follows the tiered approach by application of EUSES as a first (screening) stage. If the conservative EUSES-based risk assessment does not indicate that the PEC is less than the PNEC, the risk assessment will proceed to a higher tier. This may occur either within EUSES (*e.g.* by refining assumptions or by replacing specific EUSES predictions by experimental test data) or at a still higher tier as an extension to EUSES (*e.g.* by the inclusion of environmental monitoring data or of additional experimental test data).

2.5.1 Modifications of EUSES - Exposure

HERA incorporates modifications to some of the EUSES default parameters. The most significant modification concerns the detergent release scenario (Industry Category 5, Personal/Domestic, and Use Category 9, Detergents). HERA provides two optional modifications to the detergents scenario. *In the first, HERA uses an experimentally determined worst case European regional scenario for detergents, rather than the standard European regional scenario, defined in accordance with the 10% rule [9]. In the second, the factor of four loading to local sewage works, to account for local variability in detergent usage, is replaced by a factor of 1.5.* The experimental justification for these modifications is described further in section 2.6.

As well as the detergents scenario, some other exposure modifications involved in adapting EUSES for focused risk assessment are given below.

(a) Treatment of releases from production and formulation

HERA methodology for local releases
At the local level, chemical production plants or detergent formulation plants may be very important factors in local water quality management. Adequate waste water and waste gas treatment systems must be in place to ensure that the impact of these facilities on the local environment is acceptable.

The HERA companies (within A.I.S.E. and CEFIC) accept that it is industry's responsibility to ensure that emission standards are met at production and formulation plants. However, the local risk assessment for a plant is generally driven by specific local conditions, such as specific treatment facilities and dilution factors. Generic local scenarios are typically not applicable to the individual plant situations. Instead, environmental safety should be assessed on a case-by-case basis for individual plants, and be compatible with local water quality management schemes. For this reason, it was decided not to include the local environmental risk assessments for these facilities within the scope of HERA.

HERA methodology for regional releases
Although local releases due to production and formulation facilities are outside the scope of HERA, the amount of a substance released during production and formulation processes is effectively included in the HERA regional release scenario, as specified below.

The HERA methodology assumes that, for ingredients of A.I.S.E. products used in the home and disposed of to sewer, the contribution of releases from production and

[9] European Commission Doc. ECB4/TR2/98. Draft Technical Recommendation TGD, Chapter 3, Section 2.3.8. The use of the 10% rule in emission estimations. 1 Sept 1998.

formulation processes to the total chemical released to the EU region is very small (see below) when compared to the releases to the environment after use. In EUSES and the Technical Guidance Document, this use is specified by IC5, UC9 (Personal/Domestic Use, Surfactants and Cleaning Agents). This use pattern is covered by an Emission Scenario Document, which covers IC5 and also IC6 (Public Domain) - (Technical Guidance Document, Part IV, Chapter 7, Emission Scenario Document, p.645).
The TGD Emission Scenario Document for IC5 and IC6 proposes that, as a default for HPV detergent and household cleaning substances, 0.3% of the substance produced in the EU is released to water, and 0.001% of the substance produced is released to air. This applies to a batch process – substances produced with continuous production release < 0.1% to water, as a default. The tonnage released will enter the calculation for the EU region.

Regional releases based on production volumes
The TGD Emission Scenario Document uses the production tonnage, adjusted for exported and imported quantities of the substance, as the basis for calculating the tonnage released during formulation and use. In HERA, it is assumed initially that imported volumes and exported volumes of a substance are equal, when production volumes are used to calculate the total release to the environment. HERA assumes that all material produced is ultimately released to the environment, either through losses in the formulation process, or through losses during use. Therefore, the total environmental release will be the sum of the release during production (0.3% of the production volume) and the total production volume, as all other losses due to formulation and use are already included in the production figure. The HERA tonnage input to EUSES thus should be 100.3% of the production volume. Considering the accuracy of the production figures and of the overall environmental risk assessment process, 100% of the production volume is taken for environmental release, *via* the “use” phase, in HERA.

Regional releases based on market data
If the tonnage of a substance used in detergent and household cleaning applications is determined from product formulation data and sales volumes, then releases from formulation and production facilities should be added to the tonnage thus determined to obtain a suitable HERA input tonnage value. Guidance on this process can be obtained from the TGD Emission Scenario Document, which proposes that, as a default for HPV substances, the substance formulated in the region is released to water, air, and solid waste as shown in Table 2.1.

Table 2.1 Regional releases from detergent products according to TGD

	Regular Powder	Compact Powder	Liquid
% Water	0.01	0.01	0.09
% Air	0.02	0.02	0.002
% Solid Waste	0.73	0.81	0.32

It can be seen that, as a worst case, the TGD defaults assume that 0.3% of the production tonnage of a substance is released to the region during production, and 0.84% of the tonnage formulated is released during formulation. Note that most of the material released as solid waste is sent to landfill, and thus does not figure further in the EUSES program.

As a maximum, the TGD defaults suggest that just over 101% of the tonnage of the substance formulated is released to the environment during production, formulation,

and use. The HERA input can be adjusted to reflect this value, if formulation tonnages are used as the basis of a HERA environmental risk assessment.

Regional estimation if imports/exports are significant
If either imports or exports of a substance are substantial, they will need to be taken into account explicitly in the HERA environmental risk assessment. In these cases the HERA assessments will follow the guidance given in the TGD and outlined above. The necessity to include imports and exports will be decided on a substance by substance basis, using the knowledge and expertise of the producing and formulating companies in the specific Substance Teams.

Regional estimation for substances used in other applications
If the major use of a substance covered by a HERA risk assessment is not in products marketed by A.I.S.E. member companies, then modifications to the regional release scenario may be required. In particular, if the major release to the environment occurs through domestic consumer use, but most of the production tonnage is not intended for domestic use, then the tonnage required specifically for detergent use may be chosen as the basis for the HERA risk assessment rather than the total production tonnage. In this case, the release to the region due to production must be increased to account for the higher total production volume, to give a more accurate overall regional release figure. In practice, this correction will be small. For example, since the default production release is 0.3% of the total production tonnage, even a 10% usage in detergent products will contribute 97% of the overall regional release volume. Each HERA risk assessment should clearly specify the treatment of production releases to the overall regional release of the substance.

Local releases due to production and formulation are outside the scope of HERA. Production and formulation are covered in the regional release scenario, in which 100% of the production tonnage enters the environment. Modifications may be required for substances in which a small amount of the overall tonnage is used in A.I.S.E. products, but this accounts for most of the release to the environment during the use phase.

(b) Use of Measured Values

In HERA, the use of measured values is advocated over model predictions. For some types of compound, data for adsorption, whether onto raw sewage, activated sludge, suspended solids, sediment, or soil, may need to be evaluated carefully if they are based on calculated or measured octanol/water partition coefficients (K_{ow} value). These include surfactants and other ionic compounds, due to their interface forming properties. Specific areas which may require the use of measured values include the following.

- In the EUSES program, the mechanism of adsorption is assumed to involve partitioning of the organic substance into the organic matter of the sorbent. Thus the adsorption coefficients K_d are calculated from K_{ow} (*via* the relationship adopted in EUSES between K_{ow} and the organic carbon-water partition coefficient K_{oc}) and the percent organic carbon in the solid matter, unless measured values for K_d can be supplied. If this adsorption mechanism is known to be inappropriate for a specific substance, then measured K_d values should be used. Note that for substances which can be ionised in the environment, the pKa should be compared with the environmental pH, to ensure that the risk assessment is carried out on the environmentally relevant substance.

- If possible, measured values for removal during model or operational sewage treatment will be used to replace the standard EUSES SimpleTreat estimation. This will almost always be necessary for surfactants, at least if the default biodegradation rate constants are employed, and for other polar or ionic molecules for which SimpleTreat was not designed to be predictive.

- Data measured in the environment should be of good quality, and should be representative of the environmental compartment intended (See ECETOC, 1999).

- Concentrations of anaerobically biodegradable chemicals found in sewage sludge can be adjusted to account for degradation in the anaerobic digester, if experimental values for removal during anaerobic digestion are available.

(c) Further Modifications

For naturally occurring chemicals, the EUSES risk assessment will be extended to consider background levels in the environment, and to place the concentration introduced into the environment *via* detergent products into the context of the naturally occurring substance concentration. This is described further in section 2.7.

In addition, modifications to EUSES which are necessary in order to accommodate chemicals for which EUSES was not primarily intended, such as inorganic or ionic chemicals, may also be adopted.

2.5.2 Modifications of EUSES – Effects

The ecotoxicological effects assessment is carried out in accordance with the TGD, and thus no modifications of EUSES are required. However, effects not covered in EUSES may be considered in the individual HERA risk assessments if appropriate, on a substance by substance basis. Additional environment effects which might be considered for a HERA assessment could include e. g. eutrophication or endocrine disruption, if the specific substance were considered to have the potential to cause such an effect.

2.5.3 Minimum data requirements to run EUSES within HERA assessment

The input parameters required for a complete EUSES assessment within HERA are listed below. The sensitivity of the output of the EUSES programme to these required input parameters varies, as shown in Table 2.2.

(a) Physical/Chemical Properties

- **Molecular weight**: For simple structures this can easily be determined. EUSES does not allow molecular weight ranges to be specified (*e.g.* to capture hydrocarbon chain-length distributions). An average molecular weight should suffice, at least for low tier assessments. The default input units are $g \cdot mol^{-1}$.
- **Melting point**: This number is known for most chemicals. Alternatively, a QSAR based estimate can be made. The default input units are °C.
- **Vapour pressure at 25°C**: This number is known for most volatile chemicals. The default units are Pascals.

- **Octanol-water partition coefficient**: This parameter is not strictly required by EUSES, but it is needed to obtain results for most of the assessment modules. Note that EUSES applies different ecotoxicological extrapolation factors for different classes of octanol-water partition coefficients. Log K_{ow} is the default input parameter.
- **Water solubility**: Default input units are $mg \cdot l^{-1}$. EUSES generates a flag if the predicted concentration is in excess of the aqueous solubility. Note that, for some substances, experimental data (ecotoxicity, biodegradation) may have been obtained for aqueous dispersions or other preparations containing the substance at concentrations above the level of solubility. The reported aqueous solubility may also refer to a dispersion or other non-molecularly solubilised preparation. Care should always be taken that the experimental data refer to molecularly solubilised, bioavailable material.

Table 2.2. Sensitivity of EUSES output to the required input parameters

Input Parameter	Sensitivity of EUSES Program
Molecular weight	Low
Melting point	Low – indicates liquid (m. p. < 25°C) or solid substance
Vapour pressure	Order of magnitude is important for volatile chemicals
Octanol-water partition coefficient	Significant. Best if this can be replaced by measured removal or adsorption data.
Water solubility	A flag appears if the predicted concentration exceeds the aqueous solubility
Volume of chemical produced	Significant – and linear
Degradation and transformation rates	Significant
Effects data	Significant. Linear response to PNEC.

(b) Chemical Tonnages

Total tonnage in continent: The minimum input for the exposure assessment is the actual tonnage of the chemical which is released to the environment in Europe.

(c) Degradation and transformation rates

Based on only a statement regarding the **ready biodegradability of a substance**, EUSES can develop estimations needed for the exposure assessment. The extrapolation procedures in EUSES and in the TGD can be conservative. Biodegradation rates and removal information in sewage treatment and in the environment may need to be provided at higher tiers of the risk assessment.

(d) Ecotoxicity

EUSES is designed to operate with Base Set data. If no data are entered, no effects assessment can be made.

- For the WWTP assessment, at least **one WWTP effects value** is needed. This assessment is completely separate from the aquatic / soil / sediment assessment.
- For the aquatic + sediment assessment, at least **one aquatic effects value** is needed. Sediment effects are extrapolated from the aquatic values. Note that although EUSES can run with one aquatic toxicity value, the TGD requires three values from three different trophic levels for environmental effects assessment.
- When specific effects data for soil are not available, these are extrapolated from the aquatic data. Hence, for soil, either at least one aquatic value or at least one soil value is required.
- Alternatively, PNEC values can be entered directly. In this case, no effects data need to be entered into EUSES.

Note that, for many of the input parameters listed above, special care will need to be exercised in determining valid measured data for sparingly soluble substances.

The HERA methodology begins with this minimum data set, and the EUSES default values, at screening level. Modifications to EUSES may be incorporated, as required, at different tiers of the HERA risk assessment process.

2.5.4 HERA input spreadsheet for EUSES

A spreadsheet has been developed to facilitate the input of relevant parameters into the EUSES program, and to ensure consistency of the modifications to the default EUSES parameter set. All parameters relevant to HERA can be entered into the spreadsheet in a user-friendly way. Next to the actual numbers, comments can be included. Subsequently, the spreadsheet converts the user's input into an EUSES Export File (.exf). Finally, the Export File can be imported into the EUSES program, and the EUSES model calculations can be run.

This spreadsheet is not used for any model calculations. All equations in EUSES are maintained unaltered. However, some specific models in EUSES may be by-passed by over-writing the model result with user-specified values. For example, EUSES normally predicts chemical removal in a waste-water treatment plant by means of the SimpleTreat model. *Via* the spreadsheet, the user can replace these default predictions with measured values, which override the EUSES estimations.

The HERA input spreadsheet incorporates the increase in the proportion of treated sewage to 80%, as accepted in the TGD revision discussions to account for the increase in sewage treatment in Europe. Other spreadsheet defaults incorporate the HERA Detergent Scenario, with 7% rather than 10% of production/use volumes released to the standard EU region, and 1.5 rather than 4 times the regional average loading for a "reasonable worst case" sewage treatment plant (see section 2.6).

A copy of the HERA input spreadsheet for EUSES is given in Appendix E. After verification, it is intended that the spreadsheet will be available to interested users *via* the HERA web site.

2.6 HERA Detergents Scenario

The HERA Detergents Scenario contains several modifications of the general EUSES default values which can be shown, based upon experimental data, to be appropriate for detergent ingredients released to the environment by general domestic use.

The TGD provides default emission scenarios for both regional and local risk assessment of detergent and household cleaning substances. These emission scenarios are conservative at two different levels:

- The regional risk assessment uses the standard EU region, defined as a "densely populated area of 200 x 200 km with 20 million inhabitants" (EEC, 1996, Part II, Section 2.3.8.7, EU, 1998). The population density in this region is 500 people per km^2, which is approximately five times the European average.

The number of inhabitants in the region corresponds with 5.4% of the total EU population. However, chemical releases into this region are assumed to be 10% of the total EU tonnage, "unless specific information on use or emission *per capita* is available" (EEC, 1996, Part II, Section 2.3.8.7, EU, 1998). This increase of the regional tonnage by a factor of 1.85 is done to take into account "reasonable worst case regions", where *per capita* detergent consumption is assumed to be higher than the EU average.

- For local risk assessment, an additional factor of 4 is included in the "B" tables for the detergent specific release scenario (IC5, UC9), to account for variation in the loads reaching specific sewage treatment facilities.

Detergents and household cleaning products are widely used by the entire European population. For those substances used at HPV tonnages, the variability in loading, both between sewage treatment plants and between regions, can be shown to be less than that assumed in the TGD emission scenario for these products (Saouter *et al*., 1998; Fox *et al*., 2000). The HERA detergent scenario has been developed to give a better estimate of exposure to HPV substances used in domestic washing and cleaning products, while still remaining conservative. It may not be applicable to some lower tonnage speciality ingredients in detergent products. In these cases, the standard EUSES scenario should be used.

In the HERA detergent scenario, the calculation of the regional tonnage has been refined using data on per capita detergent consumption in the different EU countries, and population densities in the more heavily populated EU areas of approximately EU region size. The local variability factor has also been refined, based on measurements of boron, a representative of a HPV detergent ingredient reaching sewage treatment plants (Fox *et al*., submitted to CHEMOSPHERE). These two refinements are explained in more detail below.

2.6.1 Refinement of the regional release scenario

The TGD regional release scenario assumes that 10 % of the EU production and use of a substance takes place within the standard EU region. However, the major release pathway for detergents is through use by the population. Thus population

density and per capita consumption should be used to calculate the release of detergent ingredients to the regional environment. If the average EU *per capita* detergent consumption were applied to the population of the standard EU region, only 5.4 % of the EU production tonnage would be assigned to this region. Hence, the TGD assumes the *per capita* consumption in the region is 1.85 times higher than the EU average.

A.I.S.E. detergent product consumption data for European countries are available for 1998 (see Figure 3). These show that the European country with the heaviest per head detergent consumption has less than 1.3 times the European average *per capita* detergent use, rather than 1.85 times the average as proposed in the TGD release scenario. However, the areas of several countries are larger than one EU region. It is possible that some of these countries could contain areas of the size of an EU region with high population density and consequently higher regional detergent ingredient release. In Table 2.3, some of the most heavily populated regions of Europe are listed, in order of population density. In some cases, these regions have been compiled by focusing on the major European cities, combining their population and area with enough of the surrounding population and area to approach a size of 40000 km^2. Representative population data for countries of approximately the size of an EU region are also given in the Table. Care has also been taken to include regions from the countries with the highest *per capita* detergent usage.

It can be seen from Table 2.3 that the German Land of Nordrhein – Westfalen has the highest population density for a region approximating the area of an EU region. However, the higher detergent consumption in the UK means that the highest regional detergent release will occur in London and Southeast England. If this region were scaled to the size of an EU region, 5.5% of the total EU detergent usage would take place in this region. Thus the most conservative regional release factor, based on measured population density and detergent consumption data, should be 5.5% of the EU tonnage.

A regional release of 5.5% of the production tonnage is entirely appropriate for the calculation of the **regional** PEC. However, use of this figure is not appropriate for the **local** PEC calculation, if the local sewage treatment plant is not described by the generic approach, but is located in one of the higher *per capita* consumption regions such as Spain or Italy. This is because the EUSES methodology calculates the local sewage treatment plant influent loading from a consumption figure which is based upon the tonnage used in the EU region. Although this is appropriate for, and indeed probably defines, a standard EU sewage treatment plant, the HERA methodology should reflect the highest actual *per capita* product usage, in order to be applicable to a sewage treatment plant in Italy or Spain. Thus in the HERA detergent scenario the maximum (Italian) *per capita* consumption of 1.25 times the EU average has been multiplied by the maximum regional release of 5.5%, to give a 7% regional release figure. Although this is overly conservative for the regional calculation, it will generate an appropriate *per capita* input for local sewage treatment plants in the areas of heaviest *per capita* product usage.

HERA uses 7% of the formulation tonnage as the regional tonnage, to enable the local sewage plant input to reflect the areas of highest per head consumption.

2.6.2 Refinement of the local release scenario

The local release scenario uses a *per capita* input derived from the regional tonnage, as described above. In addition, the TGD assumes that, as a reasonable worst case, four times the average amount of a detergent ingredient will reach the sewage treatment plant. This can be compared with monitoring data collected for boron, a detergent ingredient whose distribution is representative of other HPV detergent ingredients, in sewage treatment plant effluents. Because boron is not degraded or adsorbed or otherwise removed in the sewer, measurements at the sewage treatment plant inlet should reflect the amount of boron disposed to sewer. This has been demonstrated (Holt *et al*., 1998) in the UK, where regional detergent consumption figures agreed with 28 daily composite STP inlet samples, within the error of the measurement (95% confidence limits).

Table 2.3. Population densities and detergent releases for EU regions

Region	Population	Area km2	Number of EU regions	Population density	Detergent usage, kg/person/year	Regional release (Relative to EU Avg).	Proportion of EU production
Entire EU	370000000	3560000	89	104	10.06	1	0.011
Switzerland	7325000	39550	0.99	185	8.64	1.53	0.017
Madrid + All Castilla Leon population	7534000	40000	1.00	188	12.40	2.23	0.025
Cataluña (Barcelona)	6089000	32113	0.80	190	12.40	2.25	0.025
Piedemonte + Liguria	5920600	30815	0.77	192	12.61	2.32	0.026
Berlin + Brandenburg	6010000	30368	0.76	198	8.10	1.53	0.017
Bremen+ Hamburg + Niedersachsen	10200000	48771	1.22	209	8.10	1.62	0.018
Baden - Württemberg	10370000	35752	0.89	290	8.10	2.25	0.025
Belgium	10213000	32820	0.82	311	10.60	3.15	0.035
Lombardia + Veneto	13490000	42221	1.06	320	12.61	3.85	0.043
Paris, Picardie, Upper Normandie	14500000	43000	1.08	337	11.67	3.76	0.042
Campania + Lazio	11048000	30899	0.77	358	12.61	4.31	0.048
Yorkshire +Humber +North West / West Midlands	17243000	42580	1.06	405	10.02	3.88	0.043
The Netherlands	15739000	33920	0.85	464	7.44	3.30	0.037
EUSES Standard Region	20000000	40000	1.00	500			0.100
London and SE +E	**20452000**	**39794**	**0.99**	**514**	**10.02**	**4.93**	**0.055**
Nordrhein – Westfalen	17950000	34079	0.85	527	8.10	4.08	0.046

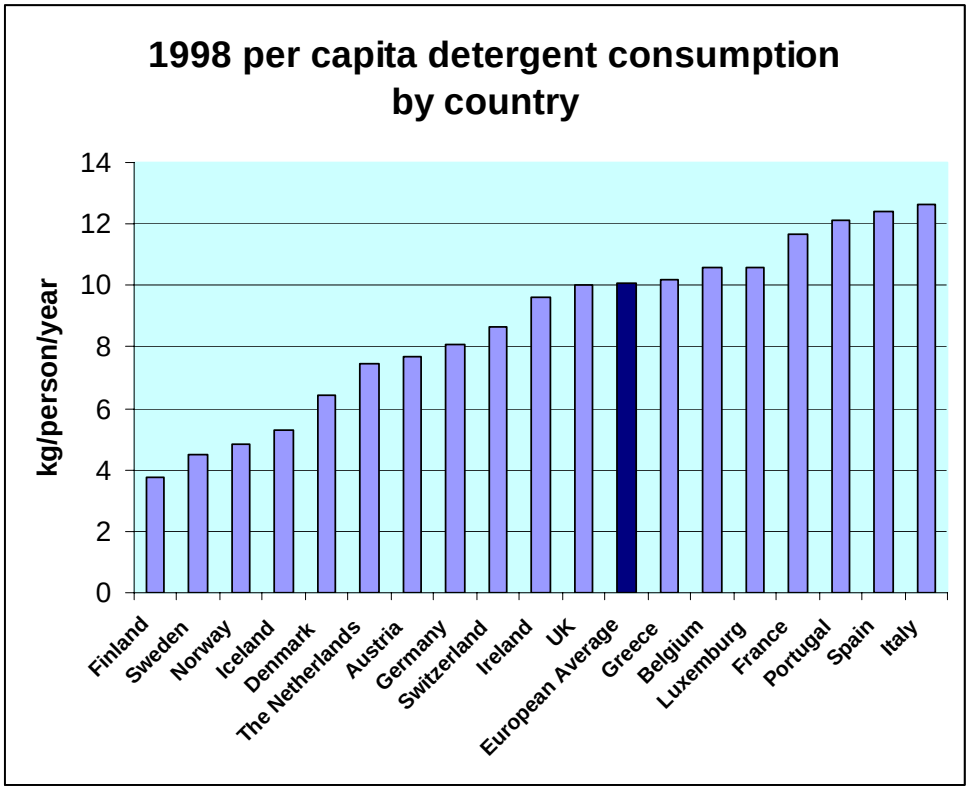


Figure 3. 1998 *per capita* European detergent consumption, per country

Boron monitoring data for 50 sewage treatment plants in four countries (UK, Italy, Germany, and the Netherlands) have been obtained which show that more than 90% of the plants receive less than 1.5 times the average predicted boron input (Fox *et al*., 2000). As the TGD (EEC, 1996, Part II, p.257) recommends that the 90th percentile of monitored exposure data be used as representative data for environmental risk assessment, this factor of 1.5 should be used for the local risk assessment of HPV detergent ingredients.

It is possible that low tonnage speciality ingredients may have greater variation in their distribution within a region, due to fashion, cost, or other factors. Thus for these ingredients, deviation from the recommended TGD factor of 4 should be justified on a case by case basis.

The TGD revision process has considered the boron data referred to above, and the current "factor of 4" will be changed to "up to a factor of 4" to reflect the appropriateness of the factor of 1.5 for HPV detergent ingredients.

The HERA detergents scenario uses a factor of 1.5 as a reasonable worst case for local chemical loading for HPV ingredients, rather than the factor of 4 used at present in the TGD.

2.6.3 Conservatism of the HERA detergent scenario

Although the regional and local emissions predicted using the HERA detergent scenario are more realistic than the default scenario recommended in the TGD, they are still conservative. This is because HERA bases regional release on the highest product release in an actual European area the size of an EU region. It then further increases this regional release, to allow EUSES to calculate a local release appropriate for treatment plants in countries with the highest *per capita* use. This gives an overly increased regional or "background" concentration, which is then added to all local PEC calculations.

It is possible that higher tiers of the risk assessment may be provided for some chemicals, to generate more accurate approximations for some of the remaining conservative assumptions. This may require the use of geo-referenced probabilistic exposure techniques, or the collection of monitoring data for some substances.

2.7 Estimation of the Environmental Relevance and Risk of Inorganic Substances used as Detergent Ingredients

Modifications to the EUSES approach are required for inorganic substances, especially those which are naturally present in the environment (*e.g.* from geological sources). The approach followed in HERA takes up some elements described in the TGD (Part 2, appendix VIII: Environmental risk assessment for metals and metal compounds) which were further developed as the "added risk approach" as described in the (draft) EU risk assessment report on zinc.

Detergent formulations may contain inorganic ingredients that also occur naturally in the environment. These will enter the aquatic environment after use of detergent products and thus contribute to the concentration in rivers. Before evaluating the possible environmental risk of inorganic chemicals according to the PEC/PNEC scheme it is necessary to put the detergent-sourced load of this inorganic into perspective. Hence, the evaluation of such chemicals should be done in a stepwise manner starting with an estimation of the detergent-based amounts/concentrations and comparing them with the total amount/concentration present in rivers. If the detergent-based use is found to be a significant source of the inorganic material (more than 10% of background – see below), then the risk assessment should proceed to a higher tier. Dependent upon the information available, the first tier of the risk assessment can be carried out using the following scheme:

A. Relevance of detergents for the environmental concentration

(a) Information required for relevance estimate:

- Detergent-relevant use figures (tonnage) of the inorganic chemical
  These may refer to a country, a region or a river catchment area. These figures may be calculated as percentages of the total tonnage based on the proportion of the EU population in the catchment area. Such data may be obtained from literature or from water authorities. Data referring to a specific river are preferred because this will establish a link to the population figures in the corresponding river catchment area. It would be very helpful if such data were available for several rivers differing in geography, size etc.

- River flow data

  Such data expressed as (*e.g.*) m^3/s need to be taken into account for calculation of the tonnages of the inorganic chemical passing through the river within a certain period, *e.g.* 1 year. The 90^{th} percentile of the flow distribution profile should be used to represent the river flow at any specific site, to reflect conditions of low flow in rivers.

(b) Calculations:

From the detergent-based usage figures referring to a specific river catchment area and the respective river flow rate, the concentration of the chemical can be calculated which results from the use in detergents. Unspecific and, thus, less reliable data for concentrations in the river can be obtained from the $PEC_{regional}$ estimates based on EUSES calculations.

(c) Relevance evaluation:

The calculated detergent-based concentration figures are to be compared with the respective measured concentrations of the chemical in rivers. This comparison allows one to evaluate whether or not the detergent-based contribution to the total concentration of the inorganic chemical in the river is significant. Although it must be acknowledged that the measured concentration in the river in most cases may already include a certain detergent-based portion, nevertheless, such a comparison will reveal if this is a major contribution or not. Ideally, measured data from unpolluted parts of a river (*e.g.* concentrations in upper reaches of a river) would provide a reliable view of the natural background concentrations. Taking account of temporal variability in river monitoring data due to natural reasons (seasonal differences, weather conditions, etc) and agriculture, it is justifiable to assume that detergent-based contributions not higher than 10% are insignificant and need no further consideration, *i.e.* no HERA assessment is warranted.

B. Risk assessment - the ‘added risk approach’

If the detergent-based contribution of the inorganic chemical to the environmental concentration is significant (> 10 % of the total concentration), the risk evaluation should be based on the 'added risk approach'. In this approach both PEC and the PNEC are determined on the basis of the added amount of the inorganic chemical resulting in an 'added Predicted Environmental concentration' (PEC_{add}) and an ‘added Predicted No Effect Concentration' ($PNEC_{add}$), respectively. The use of the added risk approach implies that only the anthropogenic amount of a substance, *i.e.* the amount added to the natural background concentration, is considered to be relevant for the effects assessment of that inorganic substance. Thus, a possible contribution of the natural background concentration to toxic effects is ignored.

The added risk approach implies

- for the exposure assessment: PEC_{add} values are to be calculated from the emission of the inorganic substance derived from use in detergents.

- for the effects assessment: $PNEC_{add}$ values are to be derived from toxicity data that are based on the added inorganic in the tests. Thus, the $PNEC_{add}$ is the maximum permissible addition to the background concentration.

- for the environmental risk assessment: evaluation of the PEC_{add} / $PNEC_{add}$ ratio.

This added risk approach, as described in the (draft) EU risk assessment report on zinc, is recommended for the HERA risk assessments of inorganic compounds when the screening exercise indicates a significant anthropogenic source.

2.8 Indirect Exposure of Humans via the Environment

Comprehensive human exposure assessments must include indirect exposure from ingredients in air, water, soil, and the food chain. Indirect exposure is defined as exposure of the consumer to an ingredient *via* the environment. Where available, measured data are used to provide the concentration in drinking water and foods. In the absence of measured data, predictions of concentrations in air, water and soil are used to predict concentrations in drinking water and food products. At the first levels of the tiered risk assessment process, EUSES, as modified for the HERA environmental risk assessment, can be used for this prediction.

(a) Air

As vapour pressures for most detergent ingredients are low, their intake *via* air can be ignored. However, this uptake pathway will be addressed for substances with a Henry's Law coefficient of 1 or greater. This cut-off value is suggested by the SimpleTreat predictions in the TGD (TGD Part II Chapter 3 Appendix II, p. 455), which show an atmospheric release during sewage treatment of less than 1% of the substance volume for substances with a Henry's Law coefficient below 1. The HERA methodology will begin with the procedure in the TGD, accepting all TGD defaults, including the description of wet and dry deposition of both gas/vapour and aerosol particles. This methodology is expected to be further developed as the HERA programme addresses volatile substances, and to incorporate appropriate advances in modelling capability. Atmospheric monitoring data will, of course, be used if it is available.

(b) Drinking water

In the absence of measured data, EUSES can provide a $PEC_{regional}$ for surface water. This represents a steady-state concentration of the substance in surface waters, and can be used to estimate the exposure concentration *via* drinking water. This screening-level method does not consider groundwater as a drinking water source, but incorporates drinking water purification factors based on K_{ow}, Henry's Law constant, and biodegradation rate, as suggested in the TGD (Part I, Chapter 2, Appendix VII). HERA uses the EUSES methodology at screening level. It is expected that higher tiers of the methodology will be developed and used as the opportunity is provided by specific case studies.

(c) Food

Reliable and relevant measured data for food (fish, milk, meat, crops) are preferable but generally lacking. The diet can be a potential source of exposure if the substance has a low solubility in water, high solubility in lipid, and is slowly metabolised.

Estimates of uptake *via* food must consider bioconcentration and biotransfer behaviour and are made from physico-chemical properties using (Q)SAR approaches. The uncertainty in these estimates can be considerable, and will vary depending on the substance. The first tier of the HERA methodology will follow the TGD defaults, as used in EUSES. Further development of the higher

tiers of the methodology is expected as appropriate specific substances are investigated.

A "cut-off" value for initial examination of dietary contributions *via* fish, milk or meat can be set at a BCF of 1000, corresponding to a log K_{ow} of 4.3, (ECETOC Technical Report No. 67. The Role of Bioaccumulation in Environmental Risk Assessment: The Aquatic Environment and Related Food Webs. Brussels, March, 1996. ISSN – 0773- 8072-67). Substances with a low lipid solubility, or with a molecular mass well above 700, or which are highly lipophilic will need to be considered individually, as will surface-active, ionisable, and polar substances. Note that the TGD (Part II, Chapter 3, p. 245) suggests that certain classes of substance with a molecular mass greater than 700 are not likely to be taken up by fish, mainly due to steric hindrance in penetrating cell membranes.

Hence, substances with BCF values below 1000 or molecular masses higher than 700 are unlikely to contribute to indirect dietary exposure, and will not be considered in terms of indirect exposure via food. At BCF and molecular mass values where bioaccumulation may be important and in the absence of substance metabolism, exposure *via* fish, milk or meat should be estimated. This will be done in the individual risk assessments, on a case by case basis.

2.9 Determination of Confidence in the HERA Risk Assessment

In the HERA risk assessment framework, "risk" is characterised by the deterministic quotient of exposure and effects (PEC / PNEC). The assumptions and data used to determine both PEC and PNEC are typically accompanied by varying degrees of variability and uncertainty. The uncertainty depends upon the tier at which the risk assessment process is being carried out. In addition, many parameters are also subject to natural variability (*e.g.* adsorption may depend upon the organic carbon content of soil, which has a wide natural range).

Uncertainty (*i.e.* lack of certainty about the exact value of specific parameters) is typically high at the lowest assessment tiers, which are *e.g.* based on QSAR estimates, single species acute toxicity data, *etc*. At higher tiers, the realism of the assessment is increased and hence the uncertainty is reduced. Natural variability, on the other hand, is inherent in the real world, and cannot be reduced by moving to higher tiers.

The combination of "true" uncertainty and natural variability will lead to a stochasticity, or a distribution of possible values, in the final risk characterisation equation (PEC/PNEC). As in this equation it is generally not possible to distinguish between uncertainty and natural variability, we will henceforth refer to this stochasticity with the term "uncertainty", using its meaning in common English rather than its technical meaning.

The key goal of HERA environmental risk assessments is to identify whether the use of specific substances in A.I.S.E. applications may potentially cause any risks to the environment. For individual substances, PEC/PNEC will be less than 1, indicating no need for further action, or a potential risk will be identified. If PEC / PNEC is less than 1, we need to be confident that the HERA assessment will adequately ensure protection of the environment.

2.9.1 Adequacy of the risk assessment: uncertainty versus *conservatism*

Uncertainty is a key aspect which determines the confidence we can have in a HERA risk assessment. Because of the tiered approach, it is not essential for the uncertainty of the assessment to be low. However, when high uncertainties are involved, all assumptions used in the risk assessment should be conservative. The higher the uncertainty, the more conservatism is needed. On the other hand, when the assumptions and the data used in the risk assessment are very accurate, there is no need for unrealistic conservatism.

The relationship between uncertainty and conservatism is illustrated in Figure 4. Data or assumptions with high uncertainty (top) should be conservative to ensure the risk assessment protects the ecosystem. In this case, the risk assessment may be "inaccurate" but, because it is conservative, this will be adequate to assess environmental safety. On the other hand, very accurate data or assumptions (bottom) need not be conservative, especially if the range of natural variability is encompassed by the data presented. When the confidence in the exposure and effects assessments is very high, a small degree of conservatism will ensure an adequate environmental safety assessment.

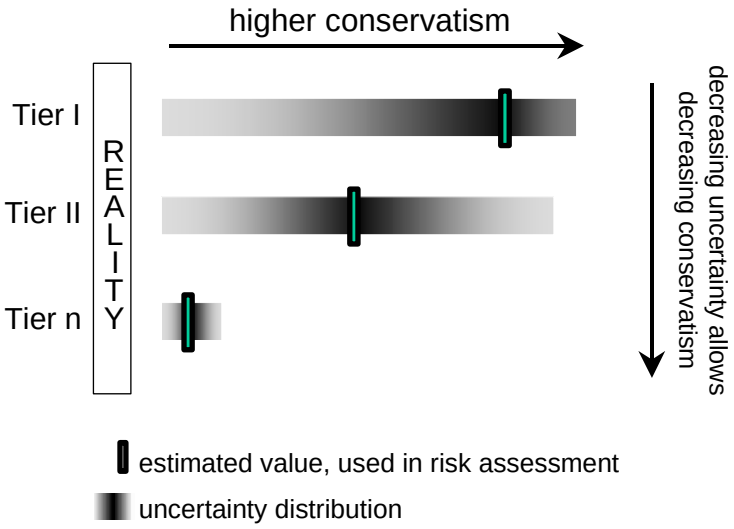


Figure 4. Relationship between required conservatism and uncertainty.

As an example to illustrate this concept, consider the assessment of removal of a substance in a sewage treatment plant. At the first tier of the assessment, the EUSES default model SimpleTreat is used. There is a significant uncertainty about (and variability of) many parameters that are inputs to this model, and the model itself over-simplifies the complex processes which occur during sewage treatment. Thus the calculated percentage removal is not expected to be accurate. However, as the SimpleTreat model's default assumptions are quite conservative, the inaccurate percentage it calculates for removal is still adequate for (low-tier) risk assessment purposes. At the other end of the scale, field monitoring data from many operational sewage treatment plants can be used to establish a realistic percentage removal for the substance. This approach provides very realistic data, which are not conservative. However, conservatism is not required because the uncertainty is very low.

Another example is related to the effects assessment. At the initial tiers, the worst-case toxicity study may be used to determine the PNEC (for example, by applying a factor of 1000 to the lowest of three acute ecotoxicity data). If the quality of this study is doubtful, the uncertainty of the PNEC is high. However, because the toxicity number is the most conservative one that exists, and also because of the magnitude of the application factor, the uncertain PNEC may still be adequate. On the other hand, if a very advanced and realistic effects assessment approach is used (probabilistic, mesocosm), the level of uncertainty is lower. Hence, due to the higher reliability and accuracy of the studies, a lower application factor is justified.

2.9.2 Uncertainty of the risk assessment

As HERA uses the EUSES program, the overall uncertainty will contain the inaccuracies and uncertainties inherent in EUSES (Schwartz *et al*., 2000; Jager, 1995; Etienne *et al*., 1997), plus additional uncertainties introduced or reduced (see section 2.6 for the detergent scenario) by the focused risk assessment methodology. The major sources of inaccuracy include the determination of the amount of the chemical that may enter the environment, where uncertainty in the tonnage and variability of the tonnage with time and perhaps with location will need to be considered. HERA concentrates on substances with a major use in the detergent sector. As a worst-case assumption these should enter the "waste water – sewage treatment plant – river" route *in toto*. Thus, there is little doubt that a refined exposure assessment which applies the detergent-specific use conditions to the overall tonnage will nevertheless deliver a reasonably realistic prognosis of the total load of a substance to be expected in the environment.

Within EUSES, uncertainties are typically compounded (*i.e*. "worst case" multiplied by "worst case"). This may lead to an unnecessary level of precaution. Sensitivity analysis can be used to identify the main sources of uncertainty and to help to focus areas for further work.

For the PEC determination, the most important substance specific sources of inaccuracy involve the identity of the substance, the determination of the amount of chemical used in household detergent products, and in some situations the octanol-water partition coefficient and environmentally dependent parameters which may be derived from it. These include removal during sewage treatment and partitioning between water and other environmental compartments. Table 2.2, section 2.5.3 gives estimations of the importance of these and other required EUSES input parameters on the risk characterisation ratio. In agreement with the provisions of the TGD, uncertainty in the PNEC is reduced by the availability of chronic data.

Since the HERA methodology is a tiered one, the inaccuracy and uncertainty will decrease as additional information is provided at the higher tiers. At the higher tiers of the HERA risk assessment, results from field monitoring and model ecosystem studies or from probabilistic based effects assessments can be used, if available for specific substances.

SECTION 3 - GUIDANCE ON RISK ASSESSMENT FOR HUMAN HEALTH

3.1 HERA Risk Assessment for Human Health

The HERA methodology for Human Health Risk Assessment focuses on the chemical substances used in household detergent and cleaning products marketed by A.I.S.E. companies. Consumers are exposed to products and not typically to individual chemical substances. Hence, HERA concentrates on assessing the risk arising from the foreseeable uses of the products by the consumer, regardless of whether the use is one recommended by the formulator or not, and on those toxicity endpoints that would be of greatest concern due to consumer exposure to products containing the chemicals. Toxicity endpoints that give rise to serious adverse health effects which may be irreversible, such as cancer or reproductive effects, are always assessed so that the potential relevance of the risk to man from contact with the product can be ascertained. The HERA assessment will also address the potential risks to the consumer arising from common accidents in the home when using the product.

It is possible that the consumer may be exposed to products other than household detergent and cleaning products which also contain the substances of interest in the HERA risk assessment. These additional exposures may also be important in the overall human health risk assessment. However, at this time, the evaluation of these other product uses is beyond the scope of this initiative and the conclusions reached in the risk assessments are relevant therefore for the consumer products considered in the HERA assessments i.e. household detergent and cleaning products.

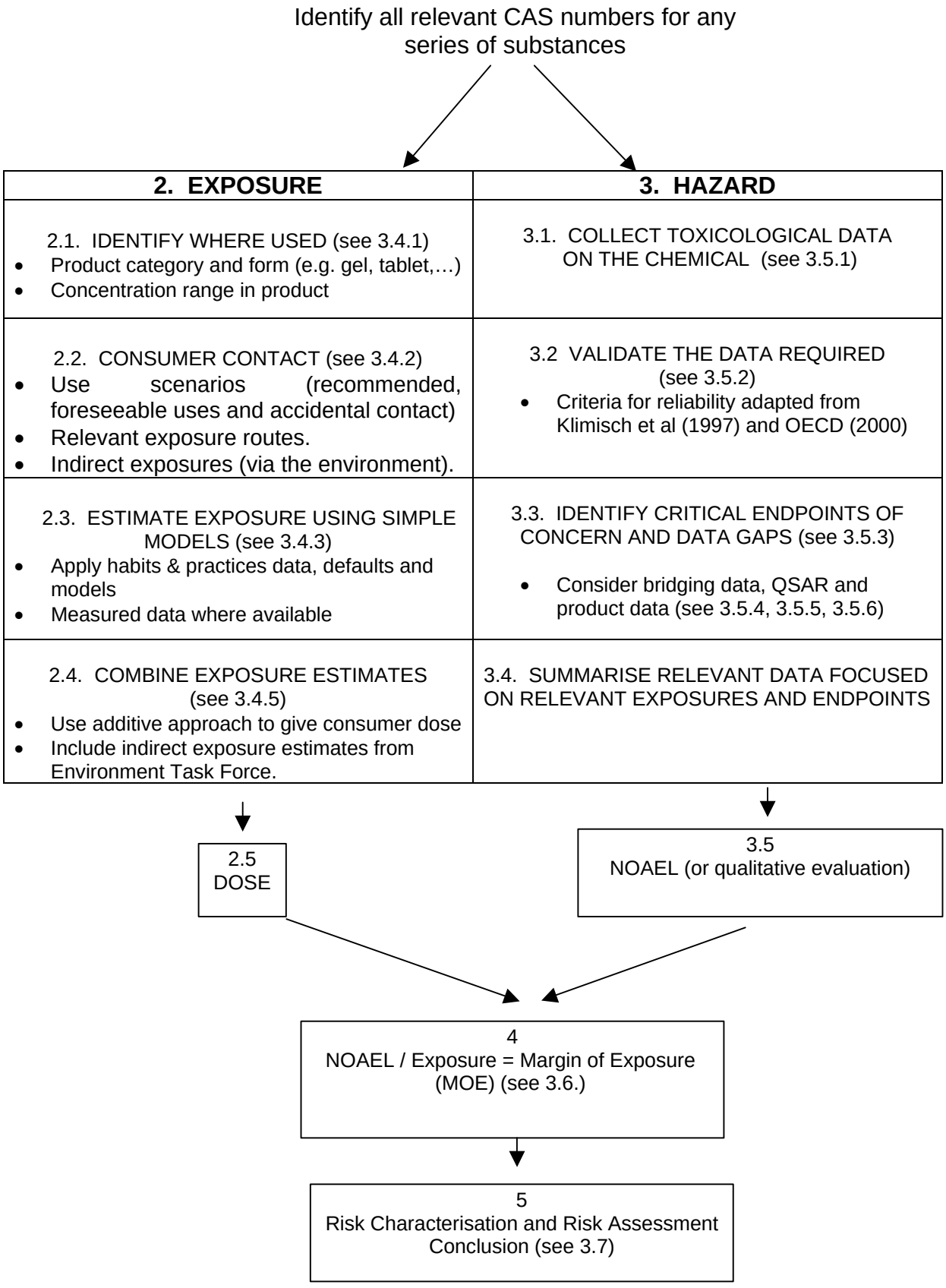
3.2 Human Health Risk Assessment Process

For the assessment of the risks posed to human health by a substance in a product, HERA follows essentially the principles and tools described in the EU Technical Guidance Document (EU TGD, 1996). Toxicity endpoints for human health are considered depending on the nature and use by consumer of the products containing the ingredient of interest, and the potential exposures that may occur from these uses. The HERA approach is tiered and is conducted in a stepwise manner until scientifically robust risk conclusions are reached. To ensure maximum transparency of the process the risk assessment report and its conclusions will be peer-reviewed and published. The overall process is summarised in the following flowchart (Figure 4) and further discussed in more detail in subsequent pages.

3.3 Chemical Substance Identification

Some criteria important for chemical substance identification have already been described in chapters 1.3.3 (a) and 2.3.

Figure 4 Overall Human Health Risk Assessment Process



3.4 Exposure

3.4.1 Use of Substance

To carry out a human health risk assessment on a chemical substance used in household detergent and cleaning formulations, it is necessary to identify those products in which the substance is used. A.I.S.E has identified a set of household product formulation categories such as fabric washing products, dishwashing products, hard surface cleaning products etc. Formulating companies will provide information on:

(1) the substance or substance class used in each of the product categories
(2) the formulation type of each of the products containing the substance
(3) the concentration range of the substance in each product type
(4) the method of use of the product
(5) exposure details – frequency of use and time of exposure

The information is sent by the formulating companies to a nominated individual in A.I.S.E in confidence and a consolidated overview of the substance, substance classes and the range of concentrations is produced. Only the consolidated information is published, so preserving the confidentiality of data from individual formulators.

3.4.2 Consumer Contact Scenarios and Exposure Routes

The exposure of consumers to a substance contained in a product is determined by the frequency and duration of use of the product and the concentration of the substance in the product. It is therefore necessary to gain an understanding of how a product is used by the consumer, and to establish the exposure route(s) of relevance to the consumer. HERA is developing a database containing detailed quantitative and qualitative data on how the consumer uses products. Such data are often referred to as habits and practices (H&P) data. These include, but are not limited to, the concentration of the product in specific use scenarios; the duration of contact between the consumer and the product for each scenario described and the frequency of product use. Possible regional differences in the habits and practices that may exist in the use of certain products will be considered.

In addition to the direct contact of the consumer with the product, HERA will also consider the potential exposure resulting from the transfer of residual product after completion of the cleaning action. For example, the transfer of substance from the residual laundry detergent from clothing to the skin, or the migration of substance from residual dishwashing product from utensils into food must also be included in the assessment of exposure.

HERA will also assess the possible uses beyond the ‘recommended product uses’ as specified by the product formulators. Product uses that may be common among consumers but do not fall within the formulator’s recommended use will be identified so that all relevant ‘foreseeable uses’ (e.g. use of a dishwashing liquid for handwashing purposes) can be addressed in the focussed risk assessment. Any potential ‘accidental’ situations that may occur in the home are also identified (e.g. splashing product into the eye), and included in the overall use scenario.

The use scenario for a substance is completed by a consideration of 'indirect' exposures via the environment, i.e. exposure to substances via intake in drinking water, food and other sources.

The purpose of the process outlined above is to identify all foreseeable sources and relevant routes of consumer contact with the product, and hence the substance in question. These scenarios will then be used to estimate the systemic exposure of consumers to the substance.

If it is found that there will be no exposure, or negligible exposure of the consumer to the product, and hence the substance of interest, for a particular route, then HERA will not carry out an exposure assessment for that route. The reasons for taking this decision will be presented so that the conclusions in the risk assessment remain transparent.

3.4.3 Consumer Exposure Calculations

The information collected as described in 3.4.2 is then used to calculate the potential consumer exposure via each relevant exposure route (dermal, oral and by inhalation). For this purpose, simple multiplicative mathematical models are used. Appendix D shows the models for dermal and oral contacts, and for contact by inhalation. The models take into account the potential for exposure to a substance for each exposure route, from the time the product package is opened until the completion of the use cycle by the consumer. Depending on the route of exposure under consideration, data may include:

(i) habits and practices data such as amount of product used, frequency and duration of use;
(ii) user data such as body weight, skin surface area, breathing rates etc.;
(iii) physical and/or chemical data on the substance or product, e.g. transfer coefficient from fabric to skin in a fabric wear scenario.

In this phase of the risk assessment, the parameters of the model equations are substituted with the appropriate data or defaults. Actual data on substances and products as provided by the suppliers and formulators are used whenever possible. Default data are only used in cases where no representative measured data for a specific parameter in the model are available.

The algorithms used to calculate the consumer exposure apply multiplications of several parameters. Some of the parameters may have wide ranges of data rather than single data points, and, in keeping with the tiered approach of HERA, a reasonable 'worst case' scenario should be first selected to calculate the exposure. However, multiplication of several of these 'worst case' estimates can lead to a significant amplification of the uncertainty, and the resulting exposure estimate may be highly unrealistic and overly exaggerated. To reduce the uncertainty in these exposure estimates if needed in a second tier, the parameters will be reviewed and the use of more realistic values considered on a case-by-case basis.

3.4.4 Consumer Exposure per route

The next step is to combine, for a given contact route, all potential exposures to a substance via different product use scenarios. Thus, for the dermal contact route, potential exposures which are identified as described above (e.g. contact *via* dishwashing solutions, laundry handwash solutions, fabric wear, surface cleaning solutions, etc.) are combined to estimate the overall skin exposure to the substance.

As noted above, if exposures to a substance occur via the environment (e.g. drinking water) or in a foreseeable rather than a recommended use scenario, then these exposure estimates need to be added to the overall estimate for a given contact route.

3.4.5 Total Consumer Exposure (all relevant routes)

Once the consumer exposure to a substance has been estimated for each relevant contact route in all product use scenarios, the maximal consumer exposure can be obtained by combining the exposures from all relevant routes.

However, the exposure estimate should not be grossly exaggerated as a result of using maximum values from worst-case scenarios that may be correlated with each other. Consumers use a range of use concentrations of laundry powder in the washing process, and vary considerably in the length of time spent washing, and in the frequency of carrying out the washing process. Expert judgement should therefore be used to evaluate the final exposure estimate from the recommended use of the product and overt conservatism should be avoided. Where necessary more realistic exposure values should be used. This process must be fully documented to maintain transparency.

Foreseeable and accidental use may be difficult to quantify. Formulating companies will be aware of many ‘non-recommended’ uses of their products by consumers, but the available data on these unusual habits and practices may not be very extensive. Thus, the uncertainty in the exposure estimates for ’other foreseeable uses’ may be greater than for estimates of normal or recommended use.

Substances used in household cleaning products are nearly all washed away from homes via the local sewage systems, and so have the potential to enter the environment. Hence consumers could be exposed ‘indirectly’ to these substances, even though they do not use the products directly. The HERA Environmental Risk Assessment Task Force will review the removal of these substances before they reach the environment. The TF will provide the Human Health Task Force with estimates of the substance in relevant environmental compartments such as air, water and the food chain. These estimates will be combined with the exposure levels calculated from the direct use of the product to obtain a complete exposure picture for the substance from its use in household cleaning products.

The total consumer exposure (both direct and indirect) is then used for comparison with the available hazard data for each endpoint of concern.

3.5 Hazard

3.5.1 Data collection

The toxicological data on each material in the HERA risk assessment process need to be collected together, so that a full hazard assessment can be made for the substance. Use will be made of data collections already available, such as the IUCLID collection of test data for materials manufactured or sold in the European Community, SIDS datasets from OECD, IPCS substance reports and those from national bodies such as BUA reports etc. Where helpful, these data sets may be supplemented with data obtained from company files. Companies will submit these data to AISE in a IUCLID format for incorporation into the database. It is not always possible to collect and display every piece of data on many of the ingredients of household cleaning products, as the literature is vast. In the case of poor quality data (see 3.5.2), or data which do not add to the overall knowledge of the substance, such information will not be included in the HERA risk assessments. Reference to all data considered will be stored in the database.

In cases where the consumer exposure is considered to be extremely low or practically impossible (e.g. due to the physical/chemical characteristics of the product form and matrix), then the hazard data for certain endpoints may not be included in the dataset. The reasons leading to this conclusion will be explained for each endpoint so that the overall process remains transparent.

3.5.2 Data validation

The Good Laboratory Practice (GLP) regulations ensure that test data produced in GLP compliant laboratories meet certain quality criteria. However, much of the data on detergent ingredients were generated before current regulatory guidelines and the GLP regulations were introduced. Hence, it is important that there is a measure of the quality of the data used in the risk assessments. It should be noted, however, that while no formal GLP systems were in existence when many of the investigations were carried out, many of the testing laboratories complied with the spirit on the regulations, and the test results should in most cases be considered as valid and robust. In addition, study results from well-described scientific publications which have been peer-reviewed can be considered to be of similar quality to guideline GLP studies. Further, if no other data exist, then data of poorer quality should be considered for individual toxicological endpoints taking the additional uncertainty in the outcome due to the lower data quality into account. Bearing in mind the aim of the EU to reduce animal testing to an absolute minimum, all available test information must be considered carefully before any significant data gaps are declared.

In 1997, Klimisch *et al*. published an article proposing a system for evaluating the quality of experimental data and publications for toxicology and ecotoxicology. The so-called reliability check is used as a first step in data validation. These criteria will be applied to data used in the focused risk assessment process of HERA. The criteria are given in Appendix C.

The complete validation process will, however include a comprehensive evaluation of the most reliable, available data for every relevant endpoint. If human experience data are used (poison control centre data, case reports, consumer/worker experience,

human volunteer studies), these should be evaluated it terms of overall relevance and with expert judgement.

While the focused risk assessment process is aimed at those ingredients used by the detergent industry, it may be necessary to consider data available on other closely related materials used by other industry sectors to strengthen the overall database or to fill in data gaps.

3.5.3 Endpoint identification

Section 1.3.3. (e) identifies where and how the products that contain the substance undergoing the risk assessment are used. Using this information, and the physical characteristics of the product (e.g. product form), it is possible to identify the following:

- The toxicological endpoints that must be addressed to evaluate the hazard of the product under the conditions of use. Hence, for a product that will regularly contact the skin, the skin irritation and sensitisation potential, and possible systemic effects as a result of dermal penetration must be considered.

- The toxicological endpoints that are of very low concern, either because of the limited exposure due to certain uses of the product or because of the latter's physical characteristics, will not be fully assessed. For example, a non-volatile material present in a solid bar product need not be considered for inhalation toxicity. In a recent document cited in the First Report on the Harmonisation of Risk Assessment procedures published by the EU Scientific Advisory Committees (October 2000), it was stated that "extremely low exposure may be considered not to represent a safety concern even in the absence of hazard identification data" (WHO).

All decisions on endpoint relevance and validity of data will be documented to ensure transparency in the final risk assessment report.

3.5.4 Considerations for the data set

One of the key features of risk process adopted by HERA is that the endpoints selected for evaluation are determined by the predicted human exposure. Exposure and consequently the hazard information that should be available for evaluation are defined by the recommended, foreseeable and accidental use patterns.

A comprehensive list of endpoints for consideration is presented in Appendix A. The principal factor dictating the need for data is relevant exposure. The risk assessor will determine which of the endpoints and data are needed for assessment.

The potential for exposure is mainly determined by:
1. the pattern of use of the product and possible routes of entry and contact with the substance
2. physical form and characteristics;
3. weight fraction of the substance in the product .

For products regularly contacting skin, the irritation and sensitisation potential and any systemic effect as a result of dermal penetration must be taken into account. When considering accidental contact with the substance from product spillage, eye irritation data need to be considered. For accidental exposures to a substance via ingestion or inhalation of products, information on acute oral toxicity and acute inhalation may be needed. In any case, it is indispensable to have information on the genotoxic potential of a substance. Information on cumulative toxicity should be considered whenever a significant repeated exposure is possible, e.g. through residues on fabrics, dinnerware or drinking water.

If exposure to a non-genotoxic substance is shown to be very low, risks of potential adverse effects after a single exposure or repeated exposures are also low. Several in-depth reviews of a large number of toxicological data sets have shown that for non-genotoxic substances, exposure levels of 1.5 µg /per person /day or below are without adverse toxicological effects (FDA, 1999; Kroes *et al*, 2000; Cheeseman *et al*, 1999; Ford *et al*, 2000; Aulmann, 1999). The chemicals included in these reviews include materials with a range of toxicological properties, including classes of substances with high acute toxicity or significant cumulative effects. In the EU, the Scientific Committee on Food has established that exposure to non-genotoxic substances in the order of 1 µg/kg bodyweight and below are without toxicological concern for the consumer. With sufficient data to confirm the lack of a genotoxic potential, the Committee does not require any toxicological data for an assessment of safety at these low levels of exposure. Where appropriate, this guidance will also be used by HERA in the human health risk assessments.

In the review of hazard data, the following toxicological information should be considered:

- acute oral and dermal toxicity
- acute inhalation toxicity *
- skin irritation
- skin sensitisation
- eye irritation
- genotoxicity
- repeated dose toxicity**
- reprotoxicity, including developmental toxicity ***
- carcinogenicity***

* May be dispensable when inhalation is unlikely (e.g. non-volatile material)
** May be dispensable for anticipated exposures below 1 µg/kg/day.
*** Relevant information should be reviewed especially when human exposures are more than negligible and there is concern from other data or SAR alerts.

Other information e.g. metabolism and human experience data with the substance or products containing the substance should also be taken into account, if available.

3.5.5 Data Summary, Data Gaps and NOAELs

The data collected in 3.5.1 should now be reviewed with respect to the relevant toxicological endpoints and where appropriate, a 'No Observed Adverse Effect Level' (NOAEL) for each of the toxicological endpoints of concern should be defined.

For some endpoints, however, such as skin and eye irritation, a NOAEL is normally not established when using guideline testing for hazard evaluation of a substance or product. Instead, the data will be assessed in a more qualitative manner, using known benchmarks. Further, study data on products containing the substance may be available that allow determination of an 'effect threshold' of eye or skin irritation for the substance in the product matrix (see 3.5.6).

The derivation of the NOAEL(s) or the description of the effects of concern for consumer exposure should be explained in a transparent way in the final report.

There may also be occasions when either the quantity or the quality of the data available for a particular toxicological endpoint are insufficient for a robust NOAEL or even a LOAEL (Lowest Observed Adverse Effect Level) to be defined. These data gaps should first be addressed by considering data available on closely related compounds, where there are demonstrable reasons to believe that interpolation is possible. This approach will be particularly important when considering surfactants, where there are many members within a homologous series, and it is unlikely that any one member will have a complete set of toxicological data.

A second approach to fill data gaps is to use any available (Quantitative) Structure Activity Relationship, (Q)SAR, algorithms or considerations. These should be used with care as QSAR human toxicology algorithms still are in the process of being fully evaluated and accepted by authorities. Nevertheless, (Q)SARs can give useful support in situations where: (i) data are scarce; (ii) the quality of the available data are below standard; and/or (iii) data are available on closely related chemicals, e.g. members of a homologous series.

3.5.6 Product Data

Many formulator companies conduct product safety assessments to reaffirm safety in use for the consumer. The process includes both theoretical assessments and experimental data generation to ensure that the toxicological properties of the product are consistent with those expected based on the characteristics of the substance of interest contained in the product (How et al., 1989). When compiling the HERA risk assessments, such product safety data may be obtained from company files, from Trade Association databases or from published reports. In particular for certain endpoints, such as skin and eye irritation, study data on products containing the substance may be available that allow a characterisation of such potential product hazards during normal and even exaggerated use. These data are valuable because they not only reflect human response after typical or extended contact with a product but they also reflect the possible influence of the other formulation ingredients on the substance of interest i.e. matrix effects.

The formulator companies participating in HERA may refer to a database of reference formulations that are available for various product categories (e.g. powder laundry detergents, hand dishwashing liquids etc.). The reference formulations are real formulations for which skin and eye irritancy test data are available (e.g. Human Patch Test, Low Volume Eye Test). Within the database, the products (which are anonymised) and the test outcomes are grouped into the respective categories (e.g. hand dishwashing product) and the individual ingredients are also grouped based on chemical and functional properties (e.g. anionic surfactants, bleach etc.). These reference formulations are regularly updated as new products and technologies are

developed. By a comparing the ingredient composition of the product formulation containing the substance of interest with a relevant reference formulation, scientifically justifiable conclusions may be made with respect to the hazard potential for the consumer of the substance of interest in the product.

Where data gaps are identified and the approaches described above (3.5.5 and 3.5.6) do not provide sufficient information as required by the risk assessor, then appropriate studies will be recommended.

3.6 Margin of Exposure (MOE)

Ultimately, the goal of a human health risk assessment is to describe, with as little uncertainty as possible, the risk, or lack of risk, to the consumer from exposure to potentially hazardous chemicals that may be contained in a variety of products.

In analogy to the environmental risk assessment, the final step in the human health risk assessment is the comparison of the human exposure estimate with a no-effect concentration or dose that has been obtained experimentally or estimated from human experience for each endpoint of concern. This is the risk characterisation step. If a no-effect level is not appropriate (e.g. skin irritant) a qualitative evaluation of the likelihood that an effect will occur at a given exposure can be made. The ratio of the no-effect level to the exposure estimate is considered and the result is called the Margin of Exposure or MOE. This ratio is also sometimes referred to as the Margin of Safety or MOS.

3.7 Risk Characterisation and Risk Assessment Conclusion

After critical review by the risk assessor, the MOE may or may not be considered to provide adequate protection for the consumer. The risk characterisation report section must give adequate consideration to the extrapolations, uncertainties and variabilities in the process of defining both the relevance of the toxicity endpoints and hazard data for man and also in the estimation of the potential consumer exposure.

The uncertainties in the process may include:

- uncertainties in extrapolating from animal data to man (interspecies extrapolation);
- uncertainties in extrapolating from less-than-lifetime exposures (exposure duration);
- uncertainties in the precision of the no effect level (precision of NOAEL);
- variability in the sensitivity of response in the human population (intra-species extrapolation);
- uncertainties in extrapolating data from one exposure route to another more relevant one (route-to-route extrapolation);
- adequacy of the overall database and relevancy of the endpoints;
- uncertainties in the assumptions used in the exposure models
- variabilities and relevance of measured data for the population exposed
- uncertainties in the overall estimate of consumer exposure i.e. in aggregating exposures from different direct and indirect sources

Expert judgement on the part of the risk assessor is required to weigh these individual parameters on a case-by-case basis. This approach, which is similar in many

respects to that used by several organisations including the EU, is a qualitative evaluation in which uncertainties are not formally accounted for in the numeric sense - they are implicit i.e. they must be considered and weighted by the risk assessor. The assumptions and arguments considered should be transparent in the risk assessment report and a justification should be provided for the conclusion reached for each endpoint of concern.

In some cases, numeric approaches to account for uncertainty and variability may be considered allowing the assessor to make use of so-called assessment or adjustment factors in the risk assessment. These factors are applied to a NOAEL or its substitute in operationally deriving a predicted no-effect dose for man. Several recent publications have reviewed the use of appropriate adjustment or assessment factors in human health risk assessment and debate and research are still ongoing (ECETOC #68, 1995; ECETOC #xx in progress).

It may be necessary to refine the focused risk assessment approach if the MOE for human health is not considered adequate. The HERA tiered approach to risk assessment allows for such refinement as follows:

- Review the hazard dataset, with the possibility of providing further data.
- Review the exposure estimates and all assumptions, with the possibility of providing more realistic measured data if needed.
- Use relevant product safety data.
- Use human experience data.

The first two procedures are a check of the data already produced to ensure that all data has been considered and that the assumptions are valid. The use of product safety data to refine the risk assessment conclusion is justified since the consumer will typically have potential for direct contact with the product. Further, there may be important matrix effects (from the other substances in the product formulation) that might influence the toxicity profile of the substance and the overall potential for harm. There are many literature references to show that a toxicological endpoint for a product is rarely the sum of the toxicity of the ingredients. For endpoints such as irritation, physico-chemical effects between the ingredients can significantly alter the toxicology of the product.

The use of human experience data may also provide important understanding and additional relevant perspective to the risk assessment. Such ‘observational’ data on man from exposure to the substances or products containing those substances may be available and could be used. The obvious advantage of considering human experience data is that the uncertainties in extrapolating animal data to man may thus become less relevant. Further, human volunteer studies conducted to the highest ethical standards may contribute additional complementary information to a risk assessment (Roggeband *et al*., 1999).

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GLOSSARY

Adequacy
Defining the usefulness of data for hazard/risk assessment purposes. When there is more than one study, the greatest weight is attached to the study that is the most reliable and relevant ("key" studies).

A.I.S.E
Association Internationale de la Savonnerie, de la Détergence et des Produits d'Entretien

Bioavailability
Refers to that portion of the total amount of a chemical that is biologically available for uptake by an organism or at a biological interface, as a result of physical and/or chemical processes.

BUA
Beratergremium für umweltrelevante Altstoffe (Advisory Committee on Existing Chemicals of Environmental Relevance).

CAS
Chemical Abstracts Service Number

Category
Is a group of closely related chemicals whose physico-chemical, ecotoxicological or toxicological properties are similar or follow a regular pattern as a result of structural similarity.

CEFIC
European Chemical Industry Council

Component
A substance consists of one or more components. In the context of EC regulation a substance normally is characterised by one set of physico-chemical and (eco)toxicological properties. However, in case the Hydrocarbon Block Method concept is applied, data sets are required for each of the blocks within the substance.(Reference – EUSES Help file.)

Conservative
Intended to ensure protection, of the human or the environment. Thus conservative data would be reasonably worst case data, and a conservative approach would combine several reasonably worst case data in a way which would err towards ensuring protection.

Continental
EUSES defines three nested areas within Europe. The continental area gives a background level of a substance which can be found in the standard EU region, before regional inputs are added. The EU region, in turn, provides the background concentration for the EU local area, which is the area in the vicinity of a local sewage treatment facility.

Detergent
Any substance or preparation which aids soil removal.

Deterministic
A deterministic calculation or process follows a specific equation. The inputs to the equation will yield a single answer or output, which will generally be a single number. Uncertainty and variability are not included in deterministic processes, though they can be added later. (See also Stochastic).

EC
Effect concentration. This is generally followed by a number, which indicates the percentage of a population which experience the effect.

EINECS
European Inventory of Existing Commercial Chemical Substances: The inventory contains a list of substances claimed to be on the European Community market between 1 January 1971 and 18 September 1981, a list of so-called "existing" substances. An EINECS number is assigned to each substance of the list.

EUSES
European Union System for the Evaluation of Substances

Exposure
The contact of a chemical, physical or biological agent with an organism

Group
See Category

Hazard
Adverse effects which a substance has an inherent capacity to cause. Hazardous properties of a substance are defined within the requirements of 67/548/EEC.

Henry's Law
The Henry's Law constant (H) relates the solubility of a chemical in water (C_w) to the partial pressure of the chemical in the gas phase (P), in the low concentration range in which this relationship is linear.

$$P\ (Pa) = H\ (Pa\ m^3 / mol)\ C_w\ (mol / m^3)$$

The partial pressure can be converted into a concentration in air (C_a) by using the ideal gas law, yielding

$$C_a = H/RT\ C_w$$

Where R is the ideal gas constant (8.314 Pa m^3 / mol K) and T is the absolute temperature (K).

HPVC (Europe)
High Production Volume Chemicals are defined as Chemicals reported to be produced or imported at levels greater than 1.000 tons per year in at least one Member State of the European Union

IPCS
International Programme on Chemical Safety, established in 1980: This is a joint programme of three co-operating organisations, ILO (International Labour Organisation), UNEP (United Nations Environment Program) and WHO (World Health Organisation), implementing activities related to chemical safety

IUCLID
The International Uniform Chemical Information Database: the basic tool for data collection and evaluation in the frame of the European Risk Assessment Programme on Existing Substances. The data structure has been designed to describe the effects of substances on human health and the environment.

K_d
Partition coefficient for adsorption of the chemical onto a specific substance – *i. e.* sewage sludge or soil. Obtained from experimental measurements by dividing the concentration of chemical adsorbed, in units of mg chemical per kg solid, by the concentration remaining in solution, in units of mg/l, to give a partition constant with units of l/kg.

K_{oc}
The partition coefficient between organic carbon and water, in units of l/kg.

K_{ow}
The octanol/water partition coefficient. This coefficient is unitless.

Local
EUSES defines three nested areas within Europe. The continental area gives a background level of a substance which can be found in the standard EU region, before regional inputs are added. The EU region, in turn, provides the background concentration for the EU local area, which is the area in the vicinity of a local sewage treatment facility.

LC
Lethal Concentration

LOEC
Lowest Observed Effect Concentration: the lowest concentration of a substance observed unequivocally to affect the test organism/s. The LOEC is generally reserved for sub-chronic and chronic studies. It is essential to observe a LOEC of a NOEC is to be described.

MOE
Margin of Exposure: Ratio of the No Observable Adverse Effect Level (NOAEL) or an appropriate substitute to the estimated or actual level of exposure to a substance.

NGO
Non Governmental Organisation: Any non-profit, voluntary citizens' group which is organised on a local, national or international level.

NOAEL
No Observable Adverse Effect Level

NOEC
No observed (adverse) effect concentration. The concentration used in a study and found to lie next below the LOEC.

Nominal concentration
The calculated concentration of a material in a medium, which has not been verified by measurement.

PEC
Predicted Environmental Concentration

pH
Negative logarithm (to the base 10) of the hydrogen ion concentration. Directly applicable to aqueous solutions, and extendable with various restrictions to other media.

pKa
Negative logarithm (to the base 10) of the acid dissociation constant Ka. Ka = [H+][A-]/[HA]

PNEC
Predicted No Effect Concentration

Preparation
A household cleaning product, as placed on the market, is, according to EU legislation, referred to as a preparation.

QSAR
Quantitative Structure Activity Relationships (QSARs) are based on a comparison of the structure or some physico-chemical property of a substance ("descriptor") with a measured endpoint which may be another physico-chemical property or a biological effect. QSARs are normally taken to mean a mathematical relationship between a descriptor and a biological or physico-chemical endpoint.

Regional
EUSES defines three nested areas within Europe. The continental area gives a background level of a substance which can be found in the standard EU region, before regional inputs are added. The EU region, in turn, provides the background concentration for the EU local area, which is the area in the vicinity of a local sewage treatment facility.

Reliability
evaluating the inherent quality of a test report or publication relating to preferably standardised methodology and the way the experimental procedure and results are described to give evidence of the clarity and plausibility of the findings (OECD, 2000)

Relevance
covering the extent to which data and tests are appropriate for a particular hazard identification or risk characterisation (OECD, 2000)

Risk
Risk is a measure of the probability that a substance (chemical) will actually cause adverse effects in a given exposure situation (scenario). It is a function of hazard and exposure.

Risk Assessment
Risk assessment is the process that evaluates the risk relative to the assessment endpoint as a result of exposure to one or more chemicals. The components include hazard identification, dose-response assessment, exposure assessment, and risk characterisation.

Risk Characterisation ratio
PEC/PNEC

SIDS
Screening Information Data Set: The data set of the OECD Existing Chemicals Programme comprises data on chemical identity, physical-chemical data, exposure information, environmental fate and pathways, ecotoxicological data and toxicological data.

Stochastic
A process which is subject to chance, and whose expression includes a mathematical description of the uncertainty of the process. (See also Deterministic). A Stocastic/deterministic process would consist of a deterministic part – i. e. an equation – and a stochastic part – e.g. applying the Monte-Carlo process to the equation, varying one or more input parameters over a specified range and distribution to produce a range of output values.

Substance/Chemical Substance/Chemical
Substances are defined as chemical elements and their compounds in the natural state or obtained by any production process, including any additive necessary to preserve the stability of the product and any impurity deriving from the process used, but excluding any solvent which may be separated without affecting the stability of the substance or changing its composition (EC Council Directive 92/32/EC; Council Regulation (EC) No. 793/93). A substance consists of one or more components. In the context of EC regulation a substance normally is characterised by one set of physico-chemical and (eco)toxicological properties. However, in case the Hydrocarbon Block Method concept is applied, data sets are required for each of the blocks within the substance. (Reference – EUSES Help file.)

Surfactant
Any material which is surface active – ie adsorbs preferentially at the air/water or the solid/water interface.

TGD
Technical Guidance Documents in support of the Commission Directive 93/67/EEC on Risk Assessment for New Notified Substances and the Commission Regulation (EC) 1488/94 on Risk Assessment for Existing Substances. EU (1996).

WWTP
Wastewater Treatment Plant (Sewage Works)

APPENDIX A – Data Requirements

The following tables allow the Supplier to assemble the required data, or as much as is available, in the approximate order in which it is required for risk assessment. Each line of data is numbered so that relationships between data may be followed in the derivation of the various inputs to the assessment. The tables also shows whether the data are needed for the environmental risk assessment (Table A.2), human health risk assessment (Table A.3) or both (Table A.1.). Essential information is given in bold. Information which is often required in practice at a higher tier of the environmental risk assessment is marked with an asterisk. Finally the table shows where further information may be obtained in this guidance document on the particular data input.

Table A.1. – General Information

Line	Item	Section of guidance document	
		Env	**Hlth**
1.	**Molecular weight**	2.6.3	
2.	**Melting point**	2. 6.3	
3.	**Boiling point**	2.6.3	
4.	**Vapour pressure at 25° C**	2.6.3	
5.	**Octanol-water partition coefficient**	2.6.3	
6.	**Water solubility**	2.6.3	
7.	***Activated sludge K_d**	2.6.1 & 2.6.3	-
8.	**K_{oc}**	2.6.1	
9.	**Total tonnage in Continent**	2.5. & 2.6.3	

Table A.2. – Environmental Data

Line	Item	Section of Guidance Document	Input considered necessary for RA on chosen substance*
10	Biotic and abiotic degradability *Specify test system/s and result/s* *a) Ready test* *b) Biodegradation in river water* *c) Biodegradation in soil* *d) Hydrolysis* *e) Photolysis*	2.6.3	
11	*****Removal in sewage treatment *% degraded *% to water *% to sludge	2.6.1 & 2.6.3	
12	Ecotoxicity – Aquatic: acute test results *Specify test system/s and result/s* *a) Algae EC_{50}* *b) Daphnia IC_{50}* *c) Fish LC_{50}* *d) Other EC_{50}*	2.6.3	
13	*Ecotoxicity – Aquatic: chronic test results *Specify test system/s and result/s* *a) Algae NOEC* *b) Daphnia NOEC* *c) Fish NOEC* *d) Other NOEC*	2.6.3	
14	Terrestrial – acute test results *Specify test system/s and result/s* *a) Plants LC50* *b) Earthworms LC50* *c) Micro-organisms LC50* *d) Other LC50*	2.6.3	
15	Terrestrial – chronic test results *Specify test system/s and result/s* *a) Plants NOEC* *b) Earthworms NOEC* *c) Micro-organisms NOEC* *d) Other NOEC*	2.6.3	
16	Micro-organisms eg in Wastewater Treatment Plants *Specify test system/s and result/s*	2.6.3	

* This column to be completed during data gathering stage.

Table A.3. – Human Health Data

Note that for human health risk assessment it may be that certain data, although given in the list, are not always needed. This is because risk assessments are made only for scenarios of relevant exposure: each scenario has its own data requirement made up of a sub-set of the data shown below.

Line	Item	Section of guidance document	Input considered necessary for RA on chosen substance
17	Acute toxicity a) Acute Oral Toxicity b) Acute Inhalation Toxicity c) Acute Dermal Toxicity d) Acute Toxicity – other routes	3.5.4.	
18	Corrosiveness/irritation a) Skin Irritation b) Eye Irritation	3.5.4.	
19	Sensitisation	3.5.4.	
20	Repeated Dose Toxicity	3.5.4.	
21	Genetic Toxicity a) in vitro b) in vivo	3.5.4.	
22	Carcinogenicity	3.5.4.	
23	Developmental Toxicity / Teratogenicity	3.5.4.	-
24	Additional Data (e.g. metabolism, skin penetration)	3.5.4.	
25	Experience with Human Exposure	3.5.4.	

APPENDIX B – HERA Report Structure

1. EXECUTIVE SUMMARY

2. CONTENTS

3. SUBSTANCE CHARACTERISATION

3.1 CAS NO AND GROUPING INFORMATION

3.2 CHEMICAL STRUCTURE AND COMPOSITION

Molecular description
Macro-molecular description (Physical State/Particle size)
Molecular weight
Melting point
Boiling point
Vapour pressure at 25° C
Octanol-water partition coefficient
Water solubility
Sorption coefficients
K_{oc}
Density
Viscosity
pH
pK_a
Oxidation

Henry's constant

3.3 MANUFACTURING ROUTE AND PRODUCTION/VOLUME STATISTICS

Total tonnage in Continent per country if possible

3.4 USE APPLICATIONS SUMMARY

4. ENVIRONMENTAL ASSESSMENT

4.1 ENVIRONMENTAL EXPOSURE ASSESSMENT

4.1.1 Environmental fate

Biotic and abiotic degradability *

a) Ready test
b) Biodegradation in river water
c) Anaerobic degradation
c) Biodegradation in soil
d) Hydrolysis
e) Photolysis

4.1.2 Removal

Removal in sewage treatment

a) % degraded
b) % to water
c) % to sludge

d) % to air

4.1.3 Monitoring Studies
- a) Water
- b) Air
- c) Soil
- d) Sewage

4.1.4 PEC Calculations
- a) PEC Water
- b) PEC Soil:
- c) PEC Sediment
- d) PEC STP
- e) Concentration in dry sewage sludge

4.2 ENVIRONMENTAL EFFECTS ASSESSMENT *

4.2.1 Toxicity

4.2.1.1 Ecotoxicity – Aquatic: acute test results
- a) Algae EC_{50}
- b) Invertebrate IC_{50}
- c) Fish LC_{50}
- d) Other EC_{50}

4.2.1.2 Ecotoxicity – Aquatic: chronic test results
- a) Algae NOEC
- b) Invertebrate NOEC
- c) Fish NOEC
- d) Other NOEC including mesocosm data

4.2.1.3 Terrestrial – acute test results
- a) Plants LC50
- b) Earthworms LC50
- c) Micro-organisms LC50
- d) Other LC50

4.2.1.4 Terrestrial – chronic test results
- a) Plants NOEC
- b) Earthworms NOEC
- c) Micro-organisms NOEC
- d) Other NOEC

4.2.1.5 Micro-organisms e.g. in Wastewater Treatment Plants

4.2.2 PNEC calculations
- a) PNEC water
- b) PNEC sediment
- c) PNEC soil
- d) PNEC stp

4.3 ENVIRONMENTAL RISK CHARACTERISATION
- a) RCR Water
- b) RCR Soil
- c) RCR Sediment
- d) RCR STP

4.4 DISCUSION AND CONCLUSIONS

5. HUMAN HEALTH ASSESSMENT

5.1 CONSUMER EXPOSURE

5.1.1 Product types: concentration (%) of the substance in product per product type

5.1.2 Consumer contact scenarios: to be defined.

5.1.3 Consumer exposure estimates

a) Detail exposure info: define S' dermal and Q' inhalatory
b) Dermal info: define C', F2, F3 and F4
c) Oral info: define M and F9
d) Inhalatory info: define C, F7 and F8
e) Other info
f) Overall exposure: dermal, oral, inhalatory, other.
g) Uptake: dermal, inhalatory and oral.

5.2 HAZARD ASSESSMENT *

5.2.1 Summary of available toxicological data

Acute toxicity

a) Acute Oral Toxicity
b) Acute Inhalation Toxicity
c) Acute Dermal Toxicity
d) Acute toxicity – other routes

Corrosiveness/irritation

a) Skin Irritation
b) Eye Irritation

Sensitization

Repeated Dose Toxicity

Genetic Toxicity

a) In vivo
b) In vitro

Carcinogenicity

Developmental Toxicity / Teratogenicity

Additional data

Experience with Human Exposure

a) Data from epidemiology
b) Data from poison control centre

5.2.2 Identification of critical endpoints

5.2.3 Determination of NOAEL or quantitative evaluation of data

5.3 RISK ASSESSMENT

5.3.1 Margin of exposure calculation

5.3.2 Risk characterisation

5.4 DISCUSION AND CONCLUSIONS

6. REFERENCES

7. CONTRIBUTORS TO THE REPORT

- Leading company
- Other contributors

For the explanation of abbreviations and signs, please, see the glossary and appendix D.

* THE SECTIONS MARKED WITH * SHOULD INCLUDE TEST DESCRIPTION WITH THE FOLLOWING INFORMATION:

- SUBSTANCE TESTED
- METHOD
- RESULTS
- CONCLUSION
- DATA QUALITY
- REFERENCES

APPENDIX C – Data Quality

General guidance concerning the scientific criteria for data selection and evaluation

Klimisch *et al*. (1997) describe a method for assessing the quality of toxicological and ecotoxicological data and propose that data evaluation be done systematically including consideration of reliability, relevance, and adequacy.

The method described in Klimisch *et al*. (1997) is similar in principle to EPA's tiered approach in that both methods present specific criteria for evaluating existing data.

Klimisch *et al*. assign a numerical value to each study for evaluating data reliability using the following scoring system:

1 = reliable without restrictions ("studies or data...generated according to generally valid and/or internationally accepted testing guidelines (preferably performed according to GLP) or in which the test parameters documented are based on a specific (national) testing guideline...or in which all parameters described are closely related/comparable to a guideline method.")

2 = reliable with restrictions ("studies or data...(mostly not performed according to GLP), in which the test parameters documented do not totally comply with the specific testing guideline, but are sufficient to accept the data or in which investigations are described which cannot be subsumed under a testing guideline, but which are nevertheless well documented and scientifically acceptable.")

3 = not reliable ("studies or data...in which there were interferences between the measuring system and the test substance or in which organisms/test systems were used which are not relevant in relation to the exposure (e.g., unphysiologic pathways of application) or which were carried out or generated according to a method which is not acceptable, the documentation of which is not sufficient for assessment and which is not convincing for an expert judgement.")

4 = not assignable ("studies or data....which do not give sufficient experimental details and which are only listed in short abstracts or secondary literature (books, reviews, etc.).")

Klimisch *et al*. (1997) describe the parameters that need to be considered to evaluate the quality of a non-standard test. The factors largely reflect those listed in the TGD (Appendix III - Evaluation of data). However, the authors do not describe the expert judgement process by which the strengths and weaknesses in the reporting of these different parameters are integrated to determine an overall quality assessment. This is also the case in the TGD where frequent reference is made to such subjective words as 'sufficient', 'adequate' and 'relatively'.

To address this limitation, the following set of quality criteria, which are a development of Klimisch *et al* (1997), should be considered in HERA data quality assessments:

- Description of the test substance
- Description of the test procedure including exposure period.
- Data on the test species and the number of individuals tested.
- Description of measured parameters, observations, endpoints.

- Control data available and acceptable according to guidelines. For some species used in environmental toxicity tests, guidelines are not available and in this instance, the guideline for the taxonomically closest equivalent species should be used.
- A dose-response has been established, except in the case of limit tests determining a NOEC/NOEL.
- Achieved dose levels/exposure concentrations were measured in the test medium or vehicle. For aquatic toxicity tests, measurements should be made at least at t_0 and t_{end} and exposure should be calculated in terms of geometric mean measured concentrations unless measured concentrations were within 20% of the nominal concentration, in which case the nominal concentrations may be used.

Any data based on a test not providing this information would be considered as less reliable compared to data from a test that was fully in line with the criteria set. Rejected test results and the reasons for their rejection will be kept in the HERA database, but only data used in the HERA environmental assessment will be justified in the HERA risk assessment report.

If available data do not conform to the quality standards, the data will be reconsidered, to determine whether any of them are acceptable under current circumstances, and in particular, that they will not underestimate toxicity. For example, in an environmental toxicity test the data could have been rejected due to an absence of measured concentrations in the test media, but for a test substance whose physical/chemical properties suggest a low potential for biodegradation / volatilisation / sorption, the data may be acceptable for screening level use in the risk assessment. The rationale for acceptance of such data must be clearly described in the risk assessment.

Irrespective of whether or not data meet the full set of quality criteria, consideration should be given as to whether the data:

- are outliers in a large data-set for a particular substance;
- fit with what is known of the toxicity of other related substances.

Most importantly, it is essential that the rationale for the expert judgement which determines the acceptability of an individual test result is clearly and transparently documented in the individual HERA substance reports.

For the environmental assessment, a probabilistic approach may be used to derive the PNEC. In this case the PNEC should be based on all chronic data of preferred reliability. Otherwise, for a deterministic assessment, the lowest of the data of preferred reliability should be used.

APPENDIX D – Consumer Exposure Models

The following algorithms allow the calculation of exposure of humans to the ingredients of AISE household cleaning products. For environmental risk assessment the algorithms embedded in EUSES are a sufficient starting point for environmental exposure, modified as described in Section 2.6 above.

(I) DERMAL

Scenario: Dermal contact to substance via product use
Outcome of equation: Systemic exposure, in *mg/kg/day*

$$EXP_{sys} = F_1 \times C' \times S_{der} \times n \times F_2 \times F_3 \times F_4 / BW$$

F_1	percentage (%) weight fraction of substance in product
C'	product load, in mg/cm^2
S_{der}	surface area of exposed skin, in cm^2
n	product use frequency, in *number of events per day*
F_2	percentage (%) weight fraction transferred from medium to skin
F_3	percentage (%) weight fraction remaining on skin
F_4	percentage (%) weight fraction absorbed via skin
BW	body weight, in *kg*

Determination of F_2

- F_2 known: enter directly into equation (I), as a percentage (%)

Note F_2 set to 100% if no medium (such as fabric, carpet) is present

- F_2 estimated from migration rate: $F_2 = m_f \cdot t$

m_f	fraction of substance migrating from article per unit time, in hr^{-1}
t	time, in *hr*

Determination of C'

(I-a) C' known: enter directly into Equation (I), in mg/cm^2

(I-b) Product directly applied onto skin

$$C' = C \times T_{der}$$

C	product concentration, in mg/cm^3
T_{der}	thickness of product layer in contact with skin, in *cm*

(I-c) Product applied to skin via fabric wash (hand, machine) and wear

$$C' = (M \times F' \times FD) / w_l$$

M	amount of undiluted product used, in *mg*
F'	percentage (%) weight fraction of substance deposited on fabric
FD	fabric density, in mg/cm^2
w_l	total weight (of fabric), in *mg*

(I-c1) percentage deposition known

$$F' = F_5$$

F_5 percentage (%) weight fraction deposited onto fabric

(I-c2) estimation of percentage deposition

$$F' = S_w / T_w$$

S_w water mass left after spin cycle or rinse, in *kg*
T_w total water mass initially present, in *kg*

(I-d) Use / knowledge of a dermal penetration coefficient

$$C' = C \times K_p \times t$$

C product concentration, in *mg/cm*^{3}

K_p dermal penetration rate, in *cm/hr*

t duration of exposure or contact, in *hr*

Note F_4 set to 100% if (I-c) is used
K_p may also be estimated from physico-chemical data, log P_{OW}, skin permeation models etc.)

(I$_{bis}$) DERMAL

Scenario: Dermal contact to substance via product use
Outcome of equation: Dermal exposure for skin sensitisation assessment, in *mg/cm*^{2} (on a *daily* basis)

$$EXP_{derm} = F_1 \times C' \times F_2 \times F_3 \times n$$

C' as determined in (I-a) or (I-b), in *mg/cm*^{2}
F_1, F_2, F_3, n as defined in Equation (I)

(II) VIA INHALATION

Scenario: Contact to substance via inhalation, following product use
Outcome of equation: Estimate systemic exposure, in *mg/kg/day*

$$EXP_{sys} = F_1 \times C \times Q_{inh} \times t \times n \times F_7 \times F_8 / BW$$

F_1	percentage (%) weight fraction of substance in product
C	product concentration, in *mg/cm³*
Q_{inh}	ventilation rate of user, in *cm³/hr*
t	duration of exposure or contact, in *hr*
n	product use frequency, in *number of events per day*
F_7	percentage (%) respirable or inhalable weight fraction of product
F_8	percentage (%) weight fraction absorbed or bioavailability
BW	body weight, in *kg*

Determination of C

(II-a) *C* known: enter directly, in *mg/cm³*, in Equation (II)

(II-b) Product used indoors for a relatively short period of time

$$C = M / V_r$$

M	amount of undiluted product used, in *mg*
V_r	room volume, in *cm³*

(III) ORAL

Scenario: Contact to substance via ingestion (accidental or per product use)
Outcome of equation: Estimate systemic exposure, in *mg/kg/day*

$$EXP_{sys} = F_1 \times M \times n \times F_9 / BW$$

F_1	percentage (%) weight fraction of substance in product
M	amount of product ingested, in *mg*
n	product use frequency, in *number of events per day*
F_9	percentage (%) weight fraction absorbed or bioavailability
BW	body weight, in *kg*

Determination of M

(III-a) *M* known: enter directly, in *mg*, in Equation (III)

(III-b) Substance unintentionally swallowed

$$M = (C / D) \times V_{app}$$

C	concentration of (undiluted) product, in *mg/cm³*
D	dilution factor *(no units)*
V_{app}	applied or ingested volume of product, in *cm³*

(III-c) Substance deposited on surface of article (dishes, utensils, glassware, etc), then swallowed (directly or via food, drink):

$$M = C'' \times S \times F''$$

C''	substance load on surface of article, in *mg/cm²*
S	surface area of article, exposed to substance, in *cm²*
F''	percentage (%) weight fraction of substance transferred from article & ingested

(III-c1) *C”* known: enter directly into (III-c), in *mg/cm²*

(III-c2) *C”* estimated from substance concentration in article

$$C'' = C_a \times T_a$$

C_a	substance concentration in article, in *mg/cm³*
T_a	“contact thickness” of article, in *cm*

(III-c3) *F”* known

$$F'' = F_{10}$$

F_{10}	percentage (%) weight fraction of substance transferred from article & ingested

(III-c4) *F”* estimated from migration rate

$$F'' = m_f \times t$$

m_f	fraction of substance migrating from article per unit time, in hr^{-1}
t	time, in *hr*

(IV) DATA SOURCE TABLE

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APPENDIX E – HERA EUSES Input Spreadsheet

Version 2.3 / 18 JULY 2000 revised 1
August 2000

HERA EUSES Input Spreadsheet

STUDY IDENTIFICATION

Study name	**name**
Study description	**description**

Author	
Institute	
Address	
Zip code	
City	
Country	
Telephone	
Telefax	
Email	

ASSUMPTIONS

General assumptions - only private use is considered
- everything goes into waste water
- emission during 365 days per year

Study-specific assumptions - list as appropriate

SUBSTANCE

General name	
Description	
CAS-No	
EC-notification no.	
EINECS no.	

		range	Note that data shown as <*x* or >*x* are sent to EUSES anything else is just for information
Molecular weight			[g.mol-1]
Melting point			[oC]
Boiling point			[oC]
Vapour pressure at 25 [oC]			[Pa]
Octanol-water partition coefficient			[log10]
Water solubility			[mg.l-1]
Activated Sludge Kd			[l/kg]
Automatically change Koc ?			[1/0]
Koc	0	(not used)	[l/kg]

TONNAGE

Total Tonnage in Continent		no HPVC	[t/y]
Percent of Continental Tonnage to Region	7%		[-] default detergent scenario: 7% of total to region
Regional Tonnage	0		[t/y] default EUSES scenario: 10% of total to region
Local tonnage increased by factor	1.5		[-] detergent scenario: 1.5 / EUSES default: 4

LOCAL CONCENTRATION

		range	
Local concentration (not including background levels)			[mg/L] enter nothing to accept EUSES local calculation

DEGRADATION AND TRANSFORMATION RATES

Biodegradability	*4*	*[0-1-2-3-4]*	used to calculate several rates (STP, soil, in-stream)

4 = not biodegradable

0 = readily
1 = failing 10-day window
2 = inherently - fulfilling criteria
3 = inherently - not fulfilling criteria
4 = not biodegradable

		range	**The lines below over-ride line 45**
Total rate constant for degradation in bulk surface water			[d-1] enter nothing to accept EUSES calculation
Total rate constant for degradation in bulk soil			[d-1] enter nothing to accept EUSES calculation
Total rate constant for degradation in bulk sediment			[d-1] enter nothing to accept EUSES calculation
Total rate constant for degradation in air			[d-1] enter nothing to accept EUSES calculation

FATE IN SEWAGE TREATMENT (CONTINENTAL and REGIONAL and LOCAL)

		range	
Accept EUSES STP model (SimpleTreat) ?	1		[1/0] enter 0 plus fractions below to override EUSES model output
Fraction of emission directed to air			[-]
Fraction of emission directed to water			[-]
Fraction of emission directed to sludge			[-]
Fraction of the emission degraded			[-]
Concentration in sludge			[mg/kg]

ECOTOXICITY

AQUATIC

		range	
LC50 algae			[mg/L] lowest values
LC50 daphnia			[mg/L] lowest values
LC50 fish			[mg/L] lowest values
LC50 other			[mg/L]

		range	
NOEC algae			[mg/L]
NOEC daphnia			[mg/L] lowest values
NOEC fish			[mg/L] lowest values
NOEC other			[mg/L]

species other		[-]

ADDITIONAL NOECS CAN BE ENTERED IN SHEET <EXF> AT B329:B344 (watch units !)

		range	
PNEC for aquatic organisms			[mg/L] enter nothing to accept EUSES approach
PNEC for sediment organisms			[mg/kg] enter nothing to accept EUSES approach

TERRESTRIAL

		range	
LC50 plants			[mg/kg]
LC50 earthworms			[mg/kg]
LC50 microorganisms			[mg/kg]
LC50 other			[mg/kg]

		range	
NOEC plants			[mg/kg]
NOEC earthworms			[mg/kg]
NOEC microorganisms			[mg/kg]
NOEC other			[mg/kg]

species name other		[-]

ADDITIONAL NOECS CAN BE ENTERED IN SHEET <EXF> AT B329:B344 (watch units !)

		range	
PNEC for soil organisms			[mg/kg] enter nothing to accept EUSES approach

WWTP MICRO-ORGANISMS

		range	
EC50			[mg/L]
specific bacterial population ?			[1/0]
EC10			[mg/L]
specific bacterial population ?			[1/0]
NOEC			[mg/L]
specific bacterial population ?			[1/0]
PNEC for WWTP microorganisms			[mg/L] enter nothing to accept EUSES approach

range: NOT sent to EUSES

name of defaults	EUSES defaults		[-]	

				default EUSES	
CONTINENTAL SYSTEM					
		range			
Area of the EU	3.56E+06		[km2]	3560000	
Number of inhabitants in the EU	3.70E+08		[eq]	370000000	
		range			
Area of continental system	*3.52E+06		[km2]	= EU minus region	*WATCH OUT: there is a bug in EUSES, which causes this number to be displayed as 100x its value (but the calculations are correct)
Number of inhabitants of continental system	3.50E+08		[eq]	= EU minus region	
Area fraction of water	0.03		[-]	0.03	
Area fraction of natural soil	0.6		[-]	0.6	
Area fraction of agricultural soil	0.27		[-]	0.27	
Area fraction of industrial/urban soil	0.1		[-]	0.1	
Water depth of system	3		[m]	3	
REGIONAL SYSTEM					
		range			
Area of regional system	40000		[km2]	40000	
Number of inhabitants of region	2.00E+07		[eq]	20000000	
Area fraction of water	0.03		[-]	0.03	
Area fraction of natural soil	0.6		[-]	0.6	
Area fraction of agricultural soil	0.27		[-]	0.27	
Area fraction of industrial/urban soil	0.1		[-]	0.1	
Water depth of system	3		[m]	3	
Fraction connected to waste water treatment	0.8		[-]	0.7	
Environmental temperature	12		[oC]	12	
Average annual precipitation	700		[mm/year]	700	
LOCAL DISTRIBUTION					
		range			
Number of inhabitants feeding one STP	10000		[eq]	10000	
Sewage flow	0.2		[m3.eq-	0.2	

			1.d-1]	
Dilution factor	10		[-]	10
Dry sludge application rate on agricultural soil	5000		[kg.ha-1.yr-1]	5000
Dry sludge application rate on grassland	1000		[kg.ha-1.yr-1]	1000

APPENDIX F – TABLE OF HABITS AND PRACTICES FOR CONSUMER PRODUCTS IN WESTERN EUROPE

TABLE OF HABITS AND PRACTICES FOR CONSUMER PRODUCTS IN WESTERN EUROPE

Developed by AISE within the HERA project in 2002

CATEGORY	Grams/Task			Use Frequency: # Tasks per week			Duration of Task		
	Min.	Max.	Typ.	Min.	Max.	Typ.			
LAUNDRY REGULAR									
Powder	55	290	150	1	18	5	Machine wash: < 1 min.		
Liquid	78	230	150	1,8	10	4	Hand wash (b): 10 min.		
LAUNDRY COMPACT									
Powder	20	200	75	1	21	5	Machine wash: < 1 min.		
Liquid/gel	40	140	90	2,8	10	4	Hand wash (b): 10 min.		
Tablet	45	135	90	3	10	4			
FABRIC CONDITIONERS									
Liquid Regular	50	140	135	3,3	10	4	Machine: < 1 min.		
Liquid Concentrate	11	90	44				Hand wash (b): 10 min.		
LAUNDRY ADDITIVES									
Powder Bleach	50	70	60				Machine: < 1 min.		
Liquid Bleach (ml)	40	100	70	1,5	4	3	Hand wash (b): 5 - 10 min.		
Tablet	20	30	25						
HAND DISHWASHING							Min.	Max.	Typ.
Liquid Regular (a)	3	10	--	3	21	14	10	45	30
Liquid Concentrate (a)	2	5	--				10	45	30
MACHINE DISHWASHING									
Powder	20	46	--						
Liquid	20	40	--	3	7	5		< 1 min.	
Tablet	20	50	--						
SURFACE CLEANERS							Min.	Max.	Typ.
Liquid (a)	30	110	60						
Powder (a)	20	40	--	1	7	2	10	20	--
Gel (neat)	20	40	--						
Spray (neat)	5	30	--				2	10	--
TOILET CLEANERS									
Powder	15	30	20						
Liquid (ml)			30	1	2	1		< 1 min.	
Gel	20	35	25						
Tablet	25	50	35						
(a) per 5 l of wash water			Min. = minimum value			Max. = maximum			Typ. = typical

volume						value				
(b) 0.1 - 1% wash solution										