Health & Ecological Risk Assessment

A Risk-Based, Product-Level Approach for Assuring Aquatic Environmental Safety of Cleaning Products in the Context of Sustainability: the Environmental Safety Check (ESC) Scheme of the A.I.S.E. Charter for Sustainable Cleaning

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ABSTRACT

Cleaning products have long been a focus of efforts to improve sustainability and assure safety for the aquatic environment when disposed of after use. The latter is addressed at ingredient level through environmental risk assessment, including in formal frameworks such as REACH. Nevertheless, in the context of programs to improve overall sustainability, stakeholders demand both environmental safety assurance and progress at product level. Current product-level approaches for aquatic toxicity (e.g., USEtox™, Critical Dilution Volume) can be seen as predominantly hazard-based. The more logical approach would be risk-based, because ecotoxicity is generally threshold-dependent and hazard-based assessment produces conflicts with risk-based learnings. The development of a risk-based approach to assess formulated products is described: the International Association for Soaps, Detergents and Maintenance Products (A.I.S.E.) Charter Environmental Safety Check (ESC), which is consistent with the scientific principles underlying REACH. This is implemented through a simple spreadsheet tool and internal database of ingredient parameters including predicted no-effect concentration (PNEC) and removal rate. A novel feature is applying market volume information for both product types and ingredients to permit a risk-based calculation. To pass the ESC check, the projected environmental safety ratio (PESR) for each ingredient as formulated and dosed (unless cleared by a published risk assessment or exempted as inherently low risk) must be less than 1. The advantages of a risk-based approach are discussed. The strengths and limitations of various possible approaches to standard-setting, product-ranking and driving continuous improvement in respect of potential ecotoxic impacts on the aquatic environment are considered. It is proposed that as ecotoxicity is generally accepted to be threshold-dependent, with no effect below the threshold, the most constructive approach to continuous improvement of sustainability with regard to ecotoxicity is to focus efforts on instances where the safety margins for ingredients as used in specific products are narrow. This necessitates a risk-based approach.

INTRODUCTION

Sustainable cleaning based on life cycle thinking

Efforts to improve the “overall” sustainability of cleaning products across the full life cycle have a long history (Stalmans et al. 1995; Saouter and van Hoof 2002; Cowan-Ellsberry et al. 2014).

Using the outcome of Life Cycle Assessment (LCA) studies that consider a wide range of different impacts, the International Association for Soaps, Detergents and
Maintenance Products (A.I.S.E.) has introduced a suite of voluntary industry initiatives in Europe to promote sustainable cleaning with focus on chemicals safety assessment, sustainability, resource efficiency and end-user information. One of the latest initiatives, the A.I.S.E. Charter for Sustainable Cleaning as originally introduced in 2005 (AISE 2005), addresses sustainability improvement at a company level, through commitment of signatories to implementing a suite of charter sustainability procedures (CSPs) to drive continuous improvement across the whole life cycle. Human and environmental safety is assured through ingredient-based risk assessment procedures for raw material qualification as well as for premarket clearance of detergents and cleaning products.

The objective of the A.I.S.E. Charter for Sustainable Cleaning is to increase the uptake by users of cleaning products that are more sustainable, and to do this across as wide a part of the sector as possible. Its approaches are thus aimed at mainstream consumers and professional users, rather than seeking to promote elite solutions likely to be adopted by only a small proportion of users. Its mandate is to be “aspirational, yet achievable by all.” The Charter is now adopted by more than 200 companies representing over 95% of European Union (EU) cleaning product output (AISE 2014a).

A priority for stakeholders that was identified through consultation following its launch was that the Charter should be developed to include a “product dimension,” that is, to identify product choices for consumers that were substantially more sustainable in life cycle terms (e.g., concentrated product formats). Consequently, the A.I.S.E. Charter for Sustainable Cleaning update 2010 (AISE 2010a) is progressively supplementing the set of CSPs with defined advanced sustainability profiles (ASPs) for individual product categories. Qualification of individual products against the ASP criteria entitles the company to display the A.I.S.E. Charter update 2010 logo on the product pack. As of October 1, 2014, ASP criteria are available for 9 major product categories covering most of the industry’s output (AISE 2010a).

Aquatic ecotoxicity and sustainability

Ensuring safety of cleaning products for the aquatic environment, to which cleaning wastewaters are ultimately discharged after use and treatment, is essential for sustainable cleaning. Safety has been demonstrated using tiered risk assessment approaches at the ingredient level through legislative frameworks such as the EU Existing Chemicals Regulation (EC 1993) and more recently the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation (EC 2006), as well as voluntary initiatives such as Human and Environmental Risk Assessment (HERA). The demand for a “product dimension” required criteria be developed to assure safety in relation to individual products.

In the context of environmental management of chemicals and chemical products, LCA and Environmental Risk Assessment (ERA) are regarded as complementary tools (Saouter and Feijtel 1999), but each approach starts from a number of different underlying assumptions. Therefore, these tools, when used for evaluation of human and environmental ecotoxicity, may give different or even contradicting results (Swedish EPA 2004). Usual Life Cycle Impact Assessment (LCIA) methods make limited use of spatial and temporal information and make use of continuous variables by following a “less is better” approach. These factors may result in a poor accordance between the expected actual impact and the impact predicted by LCIA (Potting et al. 1999). Although LCA is a comparative tool that can be used for environmental improvement of products, risk assessment is an absolute tool, which is able to predict and/or assess the occurrence of adverse effects from chemicals (Olsen et al. 2001). The role of aquatic toxicity criteria would thus be to complement life cycle-based criteria such as limits on total chemicals used, product dosage, and packaging weight.

Whereas most life cycle-based environmental indicators are treated as continuous variables, ecotoxic effects of chemicals are often associated with a threshold level and a nonlinear S-shaped relationship between dose and effect. There is a threshold level below which there is no effect, albeit that the precise level of this threshold will vary between individuals (van Leeuwen and Vermeire 2007). Managing safety assurance is mostly based on establishment of safe levels and comparison of projected exposures with those levels. For example, in the risk assessment methodologies that are the foundation of the REACH legislation (ECHA 2014a), safety for the aquatic environment is considered established when predicted environmental concentrations (PEC) in a realistic worst-case scenario fall below the predicted no-effect concentration (PNEC). The latter is conservatively derived using appropriate “assessment factors” to allow for uncertainty depending on the quality and extent of the data set.

To date, public product-level environmental assurance schemes for cleaning products have dealt with aquatic toxicity exclusively on a hazard basis. For example, the EU ecolabel criteria for cleaning products (EC 2011) are based primarily on a critical dilution volume (CDV) calculation, which does not compare exposure to safe levels. This is supplemented by restrictions on the use of ingredients with higher hazard classifications. Similarly, the USEtox™ model (Rosenbaum et al. 2008) developed to deal with ecotoxicity within LCAs, although more sophisticated than CDV, remains fundamentally hazard-based.

Hazard-based approaches, which are unrelated to safe levels, potentially conflict with the risk-based legal and organizational frameworks for ensuring that products are safe when used as intended. It can be argued that they lead to diverging and contradictory directions for formulation improvement, bring unnecessary pressure to reduce the “toxicity potential” of formulations, and conversely, could encourage products that have not been shown to be safe.

In developing the A.I.S.E. charter criteria, the challenge was thus to devise a risk-based approach for assessing individual products on the European market in terms of their...
safety for the aquatic environment in the context of sustainability improvement.

**REQUIREMENTS AND IMPLICATIONS FOR THE APPROACH**

Although the ASP criteria in the A.I.S.E. Charter update 2010 (AISE 2010a) focus on parameters that are important determinants of the life cycle impact, a specific and essential condition for qualification is that the product must pass the Environmental Safety Check (ESC) check. Because formulations are confidential, the formal check needs to be carried out by companies using a standardized approach.

The requirement thus became the development of a methodology and a simple tool (the ESC Tool), which has been developed using Microsoft Excel (compatible with version 1997–2003). The ESC Tool (AISE 2010a) enables companies to input the formulations of their products (in terms of the % content of each ingredient) and the dosage used per task, and thereby to obtain a formal pass–fail result.

The ESC methodology was required to be consistent with the established scientific principles of tiered risk assessment for the aquatic environment as embodied in frameworks such as the EU New & Existing Chemicals legislation, REACH, and HERA. Its role is to complement the above ingredient-based frameworks, giving environmental safety assurance at a product level. It needed to cover all ingredients in a formulation, whether or not yet covered by REACH, and be simple enough to be developed and launched for use on practicable timescales.

The ESC Tool makes use of an internal database of environmental parameters, covering the majority of ingredients found in cleaning products. In this respect, the Tool resembles the CDV Calculation Tool (EC 2007) that was developed for use with the EU ecoclabel scheme for cleaning products.

As the ESC check is risk-based, some additional parameters are needed, including data on per capita product consumption per category, and parameters to project total EU consumption for ingredients in all applications. The latter information is used to calculate background environmental concentrations in addition to that arising from the product being checked.

Because the ESC Check was to be a central component of the A.I.S.E. Charter for Sustainable Cleaning scheme for continuously improving sustainability, the ESC approach and Tool should be forward-looking, helping point the way to more sustainable products for the future. Consistent with the tiered approach, where readily available low-tier data may be used initially, there would need to be a mechanism for companies to use higher-tier data where necessary subject to central ratification. Similarly, mechanisms were needed to allow companies to add additional ingredients to the Tool, including new and proprietary substances, and for these too to be fully incorporated for common use following ratification.

**KEY CONCEPTS OF THE ESC CALCULATIONS**

The core of the ESC Check is a comparison of a “projected environmental concentration” for each ingredient in the formulation with the corresponding predicted no-effect concentration (PNEC) for that ingredient. Although approaches to derive the PNEC for ingredients are relatively well established, the approach to estimate environmental concentration as part of a product formulation-based approach is novel.

The environmental concentration resulting from the use of a specific commercial cleaning product depends on the sales and market share of that product. However, assessing products on the basis of their own sales volume or market share inappropriately favors products with low sales. A common basis for projecting environmental concentrations at sector level is thus required and the choice was made to project these concentrations on the assumption that the product being checked accounts for 100% of the market.

This is a conservative and challenging assumption because, in practice, different products use different ingredients to deliver the same function. It is nevertheless in keeping with the ambition for the scheme to be progressive and forward-looking: “would this formulation be safe if every product on the market used it”? This seems a philosophically sound approach to guide product development in sustainable directions.

Background environmental concentrations of an ingredient likely to arise in the environment from uses in other industries are derived using a set of conservative scaling factors based on available information on total consumption volumes and uses. This approach affords an important simplification compared to estimation via a PEC$_{\text{regional}}$ calculation (ECHA 2012a) that would need considerable additional data for each ingredient. The assumption is that, looking forward, cleaning products discharged to drain will be subject to at least secondary sewage treatment or equivalent as is already widespread practice and progressively being mandated under EU law, for example through the Urban Waste Water Treatment Directive (EC 1991).

The ESC Tool thus calculates a projected environmental concentration (ProjEC) for each ingredient, to be compared with its PNEC.

1) ProjEC = \( \frac{((\text{IngDose} \times \text{Task}) + \text{OtherUses}) \times (100 - \text{RemovalRate})}{\text{WaterUse} \times \text{Dilution} \times \text{Vol}} \)

2) IngDose = ProdDose \( \times \) IngContent%

3) Tasks = \( \frac{\text{ProductCatUse}}{\text{AvDose}} \)

4) OtherUses = CleaningUse \( \times \) \( F_{\text{ou}} \)

Where

ProjEC = projected environmental concentration at 100% market share (mg x L$^{-1}$)

IngDose = ingredient dose per cleaning task (g)

Tasks = cleaning tasks using the product category per capita per day (n)

OtherUses = ingredient down drain from other uses (g per capita per day)

RemovalRate = removal rate of ingredient during sewage treatment (%)
WaterUse = daily water use per capita (200 L standard European Chemicals Agency [ECHA] Guidance assumption)

Dilution = dilution of sewage treatment works (STW) effluent into receiving waters (10, standard ECHA Guidance assumption)

ProdDose = manufacturer’s recommended dosage of product per task (g)

IngContent = content of ingredient in the product formulation (%)

ProdCatUse = annual consumption of product category (g per capita per year)

AvDose = average dosage per task for product category (g)

CleaningUse = ingredient consumed in cleaning uses (g per capita per day)

F_{su} = scaling factor to extrapolate background release from uses other than cleaning

The challenging criterion chosen for passing the ESC Check is that the projected environmental concentration assuming 100% market share should be lower than the predicted no-effect level (PNEC). Mathematically expressed, the Projected Environmental Safety Ratio (PESR) as it is referred to, which is the projected environmental concentration at 100% market share (ProjEC) divided by the PNEC, should be less than 1

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PESR = \frac{\text{ProjEC}}{\text{PNEC}} < 1
\]

This parallels, but is more conservative than, the PEC/PNEC less than 1 criterion that is the basis for concluding no significant risk of adverse effects in the REACH legislation.

For some 50 ingredients risk assessed under HERA (covering some 250 CAS numbers) or the EU New & Existing Chemicals legislation, there is little to gain in terms of scientific understanding from performing PESR calculations. These would be more approximate. Accordingly, these ingredients are exempt from calculation in the ESC Check. Similarly, a number of substances that are intrinsically of low risk are exempted from calculation, for example those listed in Annex IV and V of the REACH Regulation (e.g., coconut oil, sorbitol) and inorganic substances that are simple salts of common ions with recognized low toxicity (e.g., sodium sulfate, potassium chloride).

Finally, there are special approaches for 3 groups of ingredients used in very small quantities, so that the scheme remains sufficiently simple and practical. Dyes are dealt with not as individual substances, as they are very numerous, but grouped into 16 groups based on a 4 x 4 matrix of PNEC ranges and removal rates commonly relevant for different types of dyes and pigments (AISE 2014b). Perfumes are assigned a “pass” result if attested by their manufacturers first as complying with all International Fragrance Association (IFRA) standards (IFRA 2014a) relating to potential environmental risks in respect of all their constituents, and second as complying in all respects concerning the manufacture, handling and supply of the fragrance with the IFRA Code of Practice (IFRA 2014b). Similarly, ancillary ingredients such as fillers and stabilizers in enzyme preparations, in which the active enzyme is less than 1% of the preparation, are assigned a “pass” result if the enzyme preparation used is so attested by enzyme manufacturers who do their own ESC checks in relation to the levels and dosage used.

KEY PRODUCT PARAMETERS FOR THE ESC CHECK

In addition to formulation and dosage data for the product being checked, the ESC Tool database contains various parameters for product categories and individual ingredients which the Tool uses in the Check calculations. The use of quantitative parameters to describe current consumption of different product types and of the various ingredients across all uses is a novel feature of the ESC approach that is essential in allowing the check to be risk-based.

Per capita consumption data for cleaning product categories

To calculate a projected environmental concentration (ProjEC) of each ingredient that might arise if the product being checked had a 100% market share, requires a parameter (ProdCatUse) to describe market volume for that product category. The parameters incorporated in the Tool database for each product category are primarily derived from data published for the German market by the German Cosmetic, Toiletry, Perfumery and Detergent Association (IKW). This was initially selected as providing a likely worst-case scenario for Europe as Germany is a large, relatively mature market where per capita product usage is expected to be high.

Average dosage per task for each product category

If all products were used at the same dosage per task, environmental concentrations arising from the product being checked could be projected directly from the per capita consumption data for the relevant product category. In some categories, however, important improvements in sustainability are being achieved by the concentration of products (van Hoof et al. 2003; AISE 2010b) thus requiring less packaging and saving on transport. The product dosage in some cases can be less than half the dosage of “standard” products. The % content of most ingredients in concentrates is higher than in “standard” products, but this is counterbalanced and often outweighed by the corresponding dosage reduction so the environmental concentrations arising are often lower.

Accordingly, each individual product is checked at its own recommended dosage, and 100% market share is effectively defined in terms of “tasks” rather than tonnage. This notion of a task corresponds to the “Functional Unit” approach used for example in ecolabel CDV calculations. An average dose per task (AvDose) is thus estimated for each category using available market data and a conservative expert assessment by the A.I.S.E. ESC Task Force that oversees the integrity of all data in the Tool.
INGREDIENT PARAMETERS IN THE ESC CHECK

A simple ESC check uses several parameters for each ingredient, these being held in the database within the ESC Tool.

Predicted no-effect concentration

Predicted no-effect concentrations, which reflect the relative toxicity of the substance to aquatic organisms, are derived following as closely as possible the standard scientific assessment procedures defined in detail in the EU Guidance for the Implementation of REACH (ECHA 2008).

Most PNEC values included in the ESC Tool database were initially based on data presented in the Detergents Ingredients Database (DID-list) 2007 compiled for use with the EU eco-label for cleaning products. However, in some cases the PNEC values have been recalculated as some PNECs in the DID-list are based on nonstandard “assessment factors” rather than those set out in Table 1.

In a limited number of cases, further refinement of PNECs has been conducted to take account of better quality data available or because initial screening trials indicated a need for refinement given the conservative assumptions in the ESC calculations. Such refinement again followed the ECHA Guidance scientific principles (ECHA 2008).

In a snapshot analysis conducted on Version 2.0 of the ESC Tool in 2012, of 117 ingredients subject to PESR calculations, 89 PNEC values in the ESC database were the same as in the DID-list, 19 were refined to a higher (less severe) value, and 9 had been assigned a lower (more severe) value.

Removal rate

The removal rate parameter defines what percentage of an ingredient would be expected to be removed during sewage treatment, thereby reducing the quantities in sewage effluent emitted to the aquatic environment. The removal rate takes into account physical, chemical and biochemical processes in accordance with ECHA Guidance principles.

The initial source of removal rate parameters was the then current “HAD-list” produced by the German Hauptausschuss Detergenzien (HAD 2014) that considers all the relevant elimination processes listed above during sewage treatment, whereas the DID-list often does not. The estimated removal rates for parent compounds take account of adsorption potential, which can be estimated on the basis of n-octanol water partition coefficient (log \( P_{OW} \)), and biodegradability, as indicated by the result of ready or inherent biodegradation screening tests (see Table 2). It should be noted that this approach to estimating removal rates is also implemented by the SimpleTreat (Version 3.1) calculation model for wastewater treatment plants described in the ECHA Guidance (ECHA 2012b).

As with the PNECs, removal rates for a limited number of ingredients have been refined, for example using data from simulated sewage treatment tests or field monitoring work, either because better quality data was known to be available or the need for that was indicated. Such refinement again followed the ECHA Guidance scientific principles. In the snapshot comparison with DID-list values in 2012 described above, 39 ingredients had the same value as the DID-list, 27 were refined to a higher (less severe) value, and 51 were assigned a lower (more severe) value.

Table 2. Removal rates based on biodegradability and log \( P_{OW} \)

| Log \( P_{OW} \) | Readily biodegradable | Inherently biodegradable | Poorly biodegradable |
|-----------------|------------------------|--------------------------|----------------------|
| <2              | 87                     | 40                       | 0                    |
| 2–4             | 90                     | 50                       | 25                   |
| >4              | 93                     | 70                       | 60                   |
| Surfactants     | 95                     | —                        | —                    |

Table 1. Assessment factors used in derivation of PNECs

| Available data                                                                 | Assessment factor |
|--------------------------------------------------------------------------------|-------------------|
| At least 1 short-term L(E)C50 from each of 3 trophic levels of the base-set (fish, Daphnia or algae) | 1000              |
| One long-term NOEC (either fish or Daphnia)                                      | 100               |
| Two long-term NOECs from species representing 2 trophic levels (fish and/or Daphnia and/or algae) | 50                |
| Long-term NOECs from at least 3 species (normally fish, Daphnia, and algae) representing 3 trophic levels | 10                |
| SSD method                                                                     | 5-1               |
| Field data or model ecosystems                                                  | Reviewed on a case-by-case basis |

PNEC = predicted no-effect concentration; SSD = species sensitivity distribution
Ingredient consumption in noncleaning applications. Ingredient consumption in uses other than cleaning products is generally researched in tonnage terms, but then conservatively extrapolated using a series of scaling factors (F_{our}, see Table 3) in relation to the projected consumption in cleaning products. This approach, which systematically inflates the quantities and thus constitutes a more challenging check, has several advantages:

- It allows for substantial market growth in all uses including cleaning, which is appropriate for guiding formulation development in sustainable directions.
- Frequent updates to record incremental market growth are not required.
- It considers background tonnages in relation to the cleaning products use and avoids unnecessarily expending effort to accurately define parameters for high volume substances where the cleaning use makes a very small contribution to environmental loads.

Once an approximate consumption tonnage is defined for an ingredient, an appropriate scaling factor is defined following the rules set out in Table 3.

As with other key parameters, tonnages are approached on a tiered basis. Most often, total consumption tonnages in all applications are used initially as an estimate for use in “other industries” as they are generally the most readily available consumption figures. This is highly conservative because the total tonnage is assumed to be discharged to sewer and because no reduction is made for the amount used in cleaning products, already counted elsewhere. Where these initial estimates need refining, data on consumption subdivided by major end uses is required: the amount actually consumed in cleaning products can be deducted from the total, and quantities consumed in other industries can be reduced pro rata to reflect the proportion likely to be discharged to sewer.

Important sources for the data include chemical market research publications and literature. The OECD ChemPortal web site (OECD 2014) provides a convenient route to a wide range of governmental and international chemical safety assessment programs that can be useful sources of tonnage data.

For ingredients in the ESC Tool database, tonnage estimates and relevant factors to reflect both cleaning and noncleaning uses respectively are derived using best available information and expert judgement by the A.I.S.E. ESC Task Force.

### USING THE ESC TOOL

The ESC spreadsheet Tool allows quick and easy routine checking of formulations even for smaller companies, initially using just the front “ESC Check Form” shown in Figure 1. Instructions for use of the ESC Tool are set out in detail in a manual on the A.I.S.E. Charter Web site (AISE 2014b). The ESC Tool assigns an “ESC number” to ingredients used in cleaning products to make entering product formulations easy. Many of the ESC ingredient numbers are the same as those in the EU Ecolabel DID-list 2007 and HAD-list, and in some cases these group similar ingredients into families. There are search facilities using either ingredient names or CAS numbers and also a text search to help users swiftly identify the relevant number.

The Tool performs PESR calculations or assigns exemptions as each ingredient is entered and the Check results are instantly available. Color coding is automatically applied (green, amber, and red) so the results are easily assessed. To pass the check, the ESC result for each ingredient in the formulation, shown in the right-hand column in Figure 1, must not be Red.

### Table 3. Calculation factors to reflect background concentration arising from other uses

| If other industries tonnage (down drain) is: | Factor (Col J) |
|--------------------------------------------|----------------|
| >5× projected category/A.I.S.E             | 10             |
| ≤5× projected category/A.I.S.E             | 5              |
| Similar to (not greater than) projected category/ A.I.S.E | 2.5           |
| Small (≤10%) compared to projected category/A.I. S.E | 1.25          |

A.I.S.E. = International Association for Soaps, Detergents and Maintenance Products.
In the fictitious example shown in Figure 1, the formulation would not pass the ESC Check because of the Red result for Ingredient 147 (PESR 1.8). It is important to emphasize that such a Red result does not indicate a risk for the aquatic environment or suggest that the product is unsafe: it simply shows that the margins of safety using the challenging conservative assumptions of the ESC approach have not been shown to be wide enough to pass the Check. An example to illustrate how the PESR calculation works in detail is set out in Figure 2.

When the Tool is being used formally as part of the process for qualifying a product under A.I.S.E. Charter update 2010, the ESC Check worksheet must be archived by the user. ESC Checks are then subject to random third-party auditing as part of the Charter procedures. The ESC Tool can of course be used informally (e.g., to explore and precheck possible future formulations).

If one or more ingredients in the formulation being checked are not already in the Tool database, the user can gather and input key parameters for the “new” ingredient and/or ingredients, again guided by the Manual (AISE 2014b). When a user has sufficient parameters in a tiered approach for the “new” ingredient to obtain a “pass” result in the Tool, before this can be considered part of a formal ESC Check for product qualification the parameters used must be notified to, and ratified by, A.I.S.E. Before they can be used for a formal Check to qualify a product, and those parameters are issued in the next version for use by all.

**ALIGNMENT OF ESC TOOL DATA WITH REACH DATA**

In 2012, the publication by ECHA (ECHA 2014b) of the first tranche of substance data gathered under the REACH regulation provided an opportunity to begin to align the ESC Tool with REACH data in line with the declared ambitions of the scheme. Data published by ECHA for substances produced in quantities of 1000 tons per annum or more (ECHA 2014b) have been systematically compared to that used to derive the corresponding parameters held in the ESC database. A repeat exercise was begun in respect of data published for a subsequent tranche of substances starting in 2014, and this is now an ongoing process periodically reviewing new data as they emerge.

This exercise has been beneficial in validating and improving the Tool, but it has also highlighted that there are shortcomings with some of the data provided in the ESC Tool.
substance dossiers on the ECHA Web site, as noted by ECHA (ECHA 2011, 2011b). Consequently, alignment of ESC parameters with REACH data must proceed cautiously. Our policy is thus to approach alignment substance by substance. Where the ECHA PNEC is lower (more severe) and soundly based the ESC value will be revised to match. Where the value seems not to be soundly based, or where further testing is planned, the ESC value will be retained until this is resolved. Where the ECHA PNEC is higher (less severe), the ESC value will not be changed unless this is known to have a direct bearing on passing the Check as regards typical formulation practice.

Of the 190 ingredients in the ESC Tool in spring 2012 when data for the first tranche of REACH substances was reasonably fully available, approximately 150 had been registered under REACH. Of these, almost half are subject to a calculation in the ESC tool: the remainder are either exempt from calculation or are dealt with in ESC as groups (e.g., major surfactant classes) rather than individual substances. Revision of the ESC PNEC to a more conservative value was indicated for 15 substances whereas for approximately 25 substances the ECHA PNEC was less severe. The ECHA dossiers for 12 substances contained no PNEC.

**DISCUSSION**

The ESC Tool is now in routine use by A.I.S.E. Charter update 2010 signatories as part of the qualification process for selected products as meeting Advanced Sustainability Profile criteria. The unique feature of the ESC approach is in bringing product category market volume and total ingredient consumption data to bear. These additional parameters allow a conservative projected environmental concentration for each ingredient to be compared to its PNEC yielding a risk-based indicator (PESR).

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Figure 2. Worked example of a PESR calculation for an ingredient in a formulation to be checked.

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| Key data applied from ESC database: |  |
|---|---|
| Dosage of product (gms/wash): | 85 |
| PNEC (Predicted No Effect Concentration): | 0.1 mg/l |
| Ingredient Number: | 49 |
| Removal Rate (in sewage treatment): 95% |
| Content Ingredient 49: | 8% |
| Tonnage used in ‘A.I.S.E.’ uses: 11,400 tpa |
| Factor ‘Total A.I.S.E.’ (similar non-A.I.S.E. use volume) = 2.5 |
| Projected background tonnage including other industries = 11,400*2.5 = 28,500 tpa |

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| Ingl. No. | Ingredient | w/w % in Formulation | ESC PNEC mg/l | Projected EC Category mg/l | PESR Category | PESR Total | PESR Total All | ESC Result |
|---|---|---|---|---|---|---|---|---|
| 46C 8/16 or C12-14 Alkyl polyglycoside | 8 | 6.6 gms/wash |
| | | 51 x 6.8 | 346.8 gms/cap/yr |
| | | 28,500 /370 million * 10^6 |
| | | 77 gms/cap/yr |
| | | 0.94 gms/person/day |
| | | 0.047 gms/person/day |
| | | 0.21 gms/person/day |
| | | 0.011 gms/person/day |
| | | 0.0235 mg/L |
| | | 0.0053 mg/L |
| | | 0.0235 + 0.0053 = 0.0288 mg/L |
| | | 0.288 / PNEC (0.1) = 0.288 |

PESR (0.288) is < 1 so ESC Check is clear for this ingredient in this product at this level.
This approach can provide positive assurance of safety for a specific product, which is important to stakeholders, in a way that hazard-based indicators cannot, because they aim for other objectives. CDV calculations for example use formulation details, PNECs, biodegradation rates and product dosages to calculate the dilution theoretically necessary to bring the environmental concentration of each ingredient below the PNEC. However, they do not compare the necessary dilution with the expected dilution, which depends on the market volume for the product type, and do not take into account concentrations arising from other uses of the ingredient.

The USEtox™ model (Rosenbaum et al. 2008) also generates a hazard indicator derived from Characterization Factors for each ingredient. These combine an Effect Factor (reflecting aquatic ecotoxicity) with Fate and Exposure Factors that together reflect what proportion of a substance emitted to various media will be available in the aquatic compartment to potentially exert a toxic effect.

The effect factors are based on HC50s that represent the concentration of an ingredient at which 50% of aquatic species will be exposed above their EC50 concentration (i.e., 50% of the population will be adversely affected or die), rather than on conservative and protective parameters such as PNECs. As the basis of indicators of relative hazard, HC50s have the advantage of lower variability that would assist comparison between ingredients. However, they describe potential for effects at relatively high concentrations (kg/m³) that are several orders of magnitude above typical PNECs (mg/L or µg/L i.e., g/m³ or mg/m³) and the environmental concentrations conservatively projected by ESC that are generally lower still.

Although risk-based assurance of safety as provided by ESC meets an important demand of stakeholders, it is both a central concept of sustainable development and a fundamental principle of the A.I.S.E. Charter for Sustainable Cleaning that sustainability should be approached on the basis of continuous improvement. It is also a common demand of stakeholders that products should be ranked in some way to allow informed choice or preference, whether that is simply by guiding consumer choice or by applying penalties or restrictions on the poorer performing.

These challenges highlight important limitations for improving sustainability in relation to potential for ecotoxic effects. The concept of continuous improvement is straightforward when dealing with continuous variables such as resource consumption. The volume of packaging used for a product for example can be incrementally reduced with some readily definable benefit. However, this needs more careful consideration when dealing with threshold-related effects such as ecotoxicity.

If cleaning products were to use ingredients at levels that caused adverse effects on the environment, such use would be unsustainable and reducing that use would be imperative. Because cleaning products are routinely shown (including by the ESC Check and the HERA assessments [HERA 2014]) to use ingredients at levels that give environmental concentrations below the PNEC so that there is no significant risk of an adverse effect, further reducing the level of use would not be expected to produce any lesser effect or tangible benefit in ecotoxicity terms.

The impossibility of reducing an effect where there is none would seem to exclude continuous improvement as regards aquatic environmental safety. Arguably, however, an ingredient that, at its customary levels of use, gives wide margins of safety is preferable in sustainability terms to one that gives only narrow margins. Clearly, there will be much less potential for growth of use when safety margins are narrow, and wide safety margins also give increased confidence that there will be no harmful effects in extreme or unusual circumstances. Moreover, to that extent that ecotoxic effects of dissimilar substances could be additive if sharing a common mode of action, the potential for such “mixture” effects will be greatest when individual substances are present in concentrations close to their individual effect levels.

PNEC derivation is inherently conservative, such that there is often a substantial margin between the PNEC and the likely effect level, but nevertheless, sustainability is arguably most likely to be improved if effort is focused on ingredients in products where the projected safety margins are narrow. The ESC calculation can highlight such instances to users, although for many ingredients, much wider margins will be able to be demonstrated through refinement of key parameters (PNEC, removal rate, use volumes) by bringing additional data to bear following the established principles of tiered risk assessment. Ingredients with extensive, high-quality data sets that display narrower safety margins represent a logical target for sustainability improvement through reformulation or development of preferable alternatives. The ESC Tool can also offer a convenient way of comparing safety margins for new ingredients, perhaps derived from “green chemistry,” against the ingredients they might replace, in the realistic context of potential formulations.

Ranking products, although intuitively attractive and a common stakeholder demand, presents numerous practical difficulties for science-based approaches. Generating metrics and scoring schemes using those metrics, against which products might be ranked, is deceptively straightforward: the question is whether the resulting rankings are coherent, valid, and consistent in terms of differentiating products that are significantly better in sustainability terms from others and indicating directions for development that accord with best science-based judgements.

As other authors have reported (van Hoof et al. 2011), scoring systems based on CDV calculations and on USEtox™ give rankings that are both qualitatively and quantitatively quite different when applied to the same set of examples of common types of laundry detergent. The authors attribute the disparities to different conceptual approaches but also point out that the differences in the calculated scores are, in fact, small compared with the uncertainty in the key parameters used.
Adding scores for individual ingredients to generate a composite or total score for a product, though operationally simple, makes the questionable assumption that environmental concentrations of dissimilar substances will invariably combine additively toward a potential toxic effect. A further difficulty here is that adding scores based on ingredient parameters (PNEC, removal rate, etc.) that are refined to different extents is not a sound approach. For example, PNECs are generally derived for purposes of risk assessment. For low toxicity substances, PNECs derived from acute data alone are frequently adequate to show no risk even though the assessment factor of 1000 applied is likely to exaggerate the assumed toxicity, possibly by orders of magnitude, versus the true level. This is not an issue for risk assessment, but it becomes one if ingredient scores are added because bias is introduced into the ranking (Pant et al. 2004).

For score addition to be sound, even if toxicity were always additive, parameters such as PNECs and removal rates on which scores are based would need to be homogeneous (i.e., refined to a similar degree). If approached through testing, the investment required would be prohibitive, and refinement of parameters for low toxicity ingredients already shown to be very safe would be unlikely to yield any real benefit.

When qualifying hurdles are set in terms of composite product scores, focus is moved further away from safety assurance because the latitude created within the overall score makes it possible for some ingredients to be used at levels that would generate environmental concentrations in excess of their PNEC.

The most fruitful approach for development of schemes to drive continuous improvement in relation to products’ potential for ecotoxic effects would therefore seem to be to focus attention selectively on ingredients where safety margins are narrow. Experience with the ESC scheme so far has shown that although participation is voluntary it has provided the incentive in a number of cases for companies to derive and obtain additional data on such ingredients.

Focusing on situations where safety margins are narrower would concentrate resources on making improvements where some tangible benefit in sustainability terms is more likely to flow from the steps taken. The determination of safety margins necessitates a risk-based approach.

CONCLUSIONS

The development of the ESC scheme provides a new, risk-based, methodology and user-friendly tool with which producers, formulators, and other stakeholders can assess the aquatic environmental safety of cleaning products to guide their sustainable development.

The scheme is in practical operation as part of the qualification of products as meeting Advanced Sustainability Profiles under A.I.S.E. Charter update 2010 (AISE 2010a). Experience of the scheme’s operation by a range of user companies has confirmed that the great majority of products can be shown to be safe for the aquatic environment with no expected adverse impact even against conservative standards and projection to 100% market share. By 2013, ESC Checks conducted with the Tool were supporting the presence of the A.I.S.E. Charter update 2010 logo on some 820 million units of cleaning product sold in Europe during the year (AISE 2013).

In the majority of cases, the PNEC and removal rate parameters used to assess ingredients in the formulations are the same or are based on the same ecotoxicological data as those in the EU ecolabel DID-list and German HAD-list. Refinement of these parameters in accordance with the principles of tiered risk assessment has been required in only a minority of cases.

This project has also shown that it is practically possible to gather information on tonnages of ingredients used in other applications and industries from a variety of sources. By using a factor-based approach that systematically inflates the tonnage, conservative projections of background concentrations in the aquatic environment can be generated to provide a robust assessment of safety. Experience of ESC Checks of a wide range of products and ingredients indicates that even substantial variations in “background” tonnage are rarely critical: where firm tonnage information is not immediately available, it is often possible to demonstrate safety using default values, minimizing the data research needed. Only in a very few cases has it proved necessary to develop estimates of cleaning product use of an ingredient by product category to eliminate the “double-counting” of that category.

Although the ESC scheme has thus been successfully implemented and is being extended progressively to other categories of products in the A.I.S.E. portfolio, it is not a substitute for full environmental risk assessments of ingredients such as have been published by the HERA program and under EU Existing Chemicals legislation. Such exercises are time-consuming, but they are both more comprehensive as well as more efficient in the long run. The prospect for extending the range of such published assessments is, however, one for the longer term as REACH registration will not be complete for substances greater than 1 tonne per annum until 2018 and does not address the important group of polymers. At that point, as volume data will still not be aggregated across all manufacturers, the ESC scheme will still provide a more complete assessment in tonnage terms and provide a standard screening check to guide manufacturers for ingredients for which there are not such detailed published assessments.

The primary driver for developing ESC was to provide a product-specific assessment and assurance of safety in response to stakeholder demands, as REACH operates at ingredient or substance level. Although risk assessment at ingredient level is adequate to assure environmental safety, product-level assessment is potentially complementary in guiding sustainable development and providing a basis for product-specific safety assurance for the consumer. For these purposes, the risk-based approach offered by ESC is preferable to hazard-based approaches as it is both more meaningful and compatible with the risk-based...
approach of the principal chemicals safety legislation such as REACH.

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Data availability—The ESC Calculation Tool, which includes all product and ingredient parameters non-specific to the formulation being checked, is available at http://www.sustainable-cleaning.com/content_attachments/documents/ESC_Calculation_Tool_Version_7_3_20151009.zip. Information and data on the broader operation of the scheme can be found at http://www.sustainable-cleaning.com/en.companyarea_documentation.orb at Section D.1.

SUPPLEMENTAL DATA

Figure S1. Schematic comparison of Hazard (CDV) and Risk-based (ESC) calculations, illustrating in detail the difference between the two approaches.

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