ENVIRONMENTAL RISK ASSESSMENT OF CHEMICALS - INDUSTRY APPROACH

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ABSTRACT

Consumer product compounds are used in homes and disposed in wastewater where they typically receive waste treatment. After treatment, sludge and effluent are released to the environment resulting in the potential exposure of terrestrial and aquatic organisms to these compounds. To ensure the environmental safety of these compounds, the environmental risk posed by chemicals released into the environment must be assessed. A reasonable, consistent and cost-effective method to conduct environmental risk assessments and to prioritize testing of these chemicals is needed which addresses risk to organisms residing in the terrestrial and aquatic compartments of the environment. This paper provides a fundamental understanding of the technical basis of environmental risk assessment using the major surfactant(i.e., LAS) used in the laundry detergent industry worldwide as a case study.

1. INTRODUCTION

There is increased environmental awareness and a desire to better understand and manage the environmental consequences of chemicals released by industry, especially chemical industry, everyday. Industry desires to effectively manage its operations so that the environment is protected. Yet, industry faces environmental issue that are numerous and complex. Moreover, there are a variety of environmental tools that often appear to compete and overlap - life cycle assessment (LCA), environmental impact assessment (EIA), environmental risk assessment (ERA), environmental audit (EA), etc.

The fundamental objectives of each of these tools are different. For example, LCA seeks to achieve efficient use of resources such as energy and materials so that emissions and wastes are reduced, whereas ERA seeks to evaluate safety or the potential for adverse effects on the environment. ERA is more developed and has been used for several years in Europe and North America.

ERA is defined as the process that evaluates the likelihood of adverse effects occurring in the environment as a result of exposure to one or more substances. Risk does not exist unless :

1. the substance has the inherent ability to cause one or more adverse effects, and
2. the substance's release into the environment is at a sufficiently high concentration and for long enough time to actually cause one or more of those adverse effects.

Environmental risk assessments are conducted to determine if a particular chemical is safe for its intended use and at its current or proposed use volume. By "safe" we mean the compound poses a low risk to organisms. In other words, the chemical : (1) is not toxic to populations of organisms at the concentrations occurring in the environment, (2) does not affect ecosystem structure and function, and (3) does not bioaccumulate or biomagnify to concentrations causing effects on organisms at higher trophic levels. Fortunately, a series of assessment or safety factors have been developed to allow the prediction of concentrations which are safe for the ecosystem from simpler laboratory toxicity studies. These assessment or safety factors are widely accepted and are used by the U.S. EPA, the European Union, and other regulatory bodies to extrapolate ecosystem level effects data from laboratory data (OECD, 1992; CEC, 1993; Nabholz et al. 1993). To date, these assessment and safety factors have not considered potential effects due to bioaccumulation and biomagnification. To address this shortcoming, bioconcentration test data are combined with a knowledge of exposure and persistence to assess the potential for exposure and effects on higher trophic level organisms. This assessment is performed in addition to the assessment for toxic effects.

Environmental risk assessment is a relatively new field having evolved from the realization in the 1970's that exposure concentrations must be kept below effect concentrations to probabilistic estimates of exposure and a refined understanding of ecologically important effects (Duthie, 1977; Cairns et al. 1979; Calabrese and Baldwin, 1993; Suter, 1994). Risk assessment is a rapidly growing science and is embraced world-wide to understand the potential impact of man's activities (e.g., pesticides, sedimentation, acid rain, thermal discharge) on the environment (U.S. EPA, 1992; CEC, 1993). Tiered risk assessment methods have been developed and applied to consumer product compounds allowing the risk to the environment of these compounds to be understood (Duthie, 1977; Beck et al. 1981).

Environmental risk assessments are conducted on individual chemicals as each chemical behaves differently in the environment due to different capacities to biodegrade, volatilize, hydrolyze, and sorb to solids. These different characteristics remove any whole product related identity necessitating assessments on individual chemicals. The assessment process we have developed contains three components which are combined into the environmental risk assessment: an exposure or fate assessment, an effects assessment, and a bioconcentration assessment.

2. ENVIRONMENTAL RISK ASSESSMENT OVERVIEW

ERA is a multiple-step process - a schematic representation is given in Figure 1. The first step is the scoping, or problem formulation step, where decisions are made on the goal, breadth and focus of assessment. This is an important step and sets the stage for the remainder of the assessment process; therefore it is extremely important that this will be done well and thoroughly. As shown in Table 1, there are four sub-components of the scoping step that involves different types of information for planning and focusing the assessment. In short, the environmental compartments (water, air, soil) into which the substance will be released or will eventually reside must be ascertained. The relative proportions that will enter into each compartment and the total amount from all uses also need to be determined. This will enable proper selection of the assessment end-points.

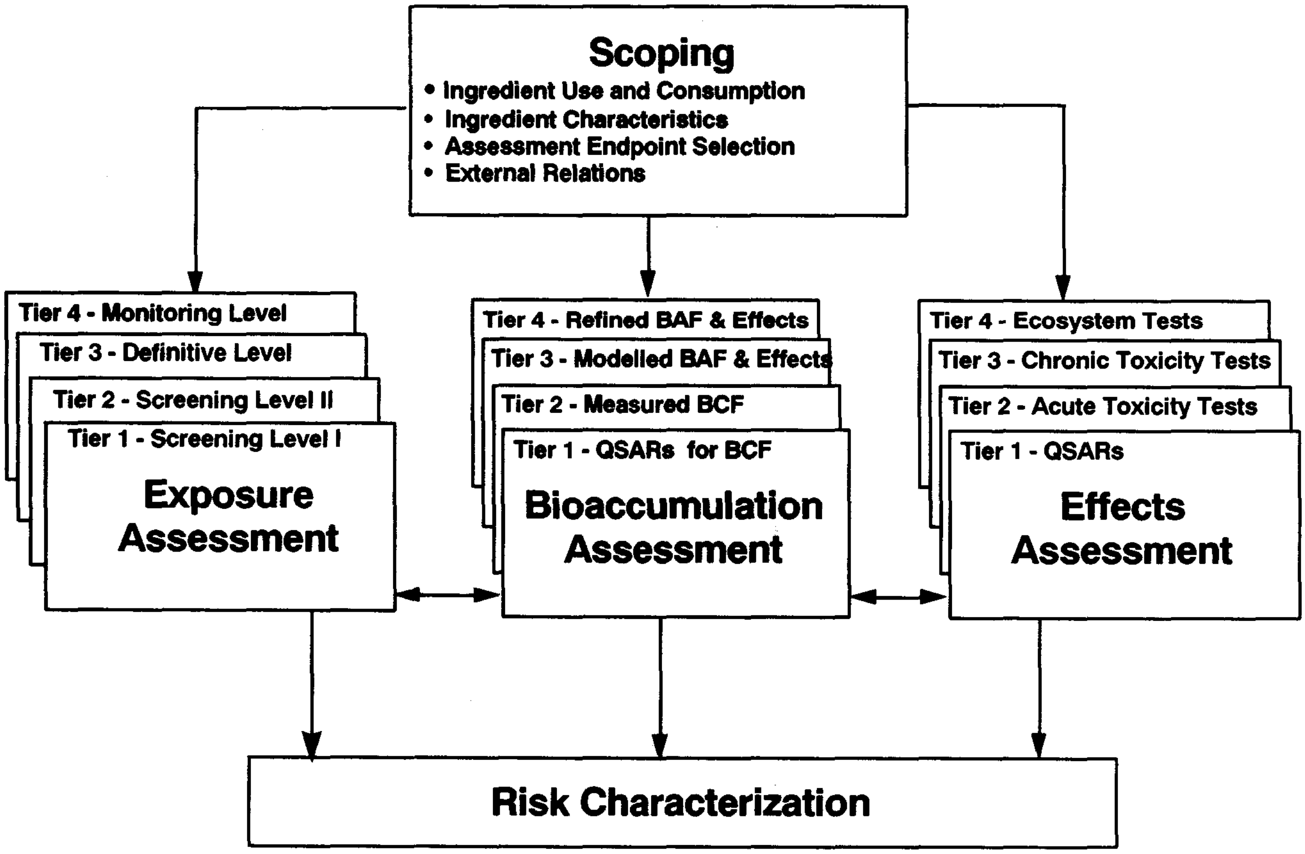

Figure 1 : Schematic representation of environmental risk assessment.

Table 1 : Sub-components of the scoping step in environmental risk assessment

Description	Examples of data / information collected	How information is used
Material Characterization	• Physical / chemical properties • Degradation potential and rate • Toxicity & bioaccumulation potential	• Determine if substance can cause one or more adverse effects • Provide understanding of the substance that is used in pathways analysis and fate assessment steps
Material Emissions	• Environmental compartments into which the material is released (e.g., water, air, soil) • Relative proportions released into each compartment • Total annual emissions from all sources • Matrix in which emission occurs	• Determine if the substance can be released to the environment and into which environmental compartments it will be released • Information used in pathways analysis and in fate assessment steps
Pathways Analysis	• Environmental characteristics and chemical properties that are most influential in determining the fate of he substance.	• Determine in which environmental compartments the substance will reside and in which risk assessments need to be conducted
Assessment Endpoint Selection	• Environmental compartments that receive the substance or in which the substance will eventually reside; importance of these environment compartments; presence of highly valued species	• Provide a benchmark against which to determine if environmental effects are occurring and likely magnitude of these effects

The second and third steps are development of two individual bodies of knowledge that must be available to conduct a risk assessment and assess safety. The first body of knowledge concerns the effect which may occur. This means collecting data on what effect a substance will cause, such as toxicity to an organism, at what concentration or dose this effect may occur, and what conditions will contribute to prevent this effect from occurring (i.e., exposure to this concentration presents an acceptably low risk of adverse effects). An *Assessment Factor* (**AF**) is used to derive the *Predicted No Effect Concentration* (**PNEC**) from the effects data. AFs account for uncertainty in estimating PNEC from the available toxicity information, as shown in Table 2 The assembly and analysis of the effects data is called a hazard of effect assessment.

Table 2 : Tiered approach to the environmental risk assessment for the aquatic environment of consumer product compounds.

EXPOSURE CONCENTRATION (PEC)	EFFECT CONCENTRATION	ASSESSMENT FACTOR	DECISION (PEC / PNEC)
Tier 1			
R = 0 D = 1 I = Calculated	QSAR, analogy or acute test, i.e., LC_{50} or EC_{50}	1,000	PEC/PNEC < 1 OK, Assessment is done Compound poses low risk PEC/PNEC > 1, continue
Tier 2			
R = Physical/chemical data and ready and inherent biodegradability tests coupled with models D = Reasonable dilution factor(s) I = Calculated	Acute toxicity tests (i.e., LC_{50} or EC_{50}) with three species, fish, invertebrate, and aquatic plant.	100	PEC/PNEC < 1; OK, Assessment is done Compound poses low risk PEC/PNEC > 1, continue

Tier 3			
R = Simulation (e.g., SCAS/CAS) D = Reasonable dilution factor(s) I = Calculated	Chronic toxicity test (i.e., NOEC) with most sensitive species identified at Tier 2.	10	PEC/PNEC < 1; OK, Assessment is done Compound poses low risk PEC/PNEC > 1, continue
Tier 4			
Environmental monitoring data obtained downstream of a wastewater treatment plant with reasonable worst case conditions of flow.	Field studies or laboratory ecosystem tests, (i.e., $NOEC_{eco}$)	1	PEC/PNEC < 1; OK Assessment is done. PEC/PNEC > 1 Risk Management

where R = removal in activated sludge wastewater treatment plant
D = dilution factor of effluent
I = influent concentration
PEC = predicted environmental concentration
PNEC = predicted "no-effect" concentration, i.e., effect concentration/ assessment factor
QSAR = quantitative structure activity relationship
LC_{50} = concentration that kills 50% of organisms
NOEC = no observable effect concentration
EC_{50} = concentration that causes effect to 50% of organisms

The second body of knowledge is understanding how exposure to the substance occurs, because effects can only occur if the exposure is sufficiently large. Evaluation of exposure involves predicting or measuring the use, discharge, distribution, degradation, and other physical /chemical properties of a substance. These data are used to calculate a *Predicted Exposure or Environmental Concentration* (**PEC**).

The final step is risk characterization, which combines the fate and effects assessment in the risk quotient, which is the ratio of the PEC and PNEC values as shown below :

$$\text{Risk} = \text{PEC} / \text{PNEC} \qquad (1)$$

If this ratio is less than one, the intended use and release of the substance is considered safe, because the environmental concentration is less than the one determined to cause no effect. If the value is greater than or equal to 1, then the assessment indicates that there is potential for adverse effect, and one of two options can be pursued. Option #1 : Reduce the uncertainty in the estimates of the PEC and/or PNEC by obtaining additional data and recalculate the risk ratio, as will be described below. Option #2 : Conduct risk management which might, for example, involve reducing the amount of the substance released to the environment. This would typically be accomplished by reducing the amount of material in product.

Fate and effects assessments are conducted in a stepwise (or tiered) and iterative manner to save costs and time, and to focus resources on those chemicals for which there is a greater need for assurance of safety. The tiered approach to risk assessment where one moves from relatively simple cost effective but conservative approaches to estimate the PEC and PNEC at initial tiers to more precise and realistic estimates of these parameters at latter tiers is illustrated in Table 2 (and Figure 3) for the aquatic environment. Once the risk quotient is below one at any tier, the risk assessment does not need to proceed further to the next level, because safety has been demonstrated.

This risk assessment process allows decisions to be made on the risk posed by a compound at the earliest time in the development of environmental data. This allows for cost effective decision-making and for resources to be allocated to those compounds having the highest risk factors. In this risk assessment process, the PEC and PNEC can be independently refined to produce the final risk assessment. This would be done if one suspected the assumptions used in one of these assessments was too conservative. Hence, one could decide based on cost and uncertainty whether to refine the PEC, the PNEC, or both.

In addition to the above, there are certain fate properties, viz., persistence and high bioaccumulation potential, that scientists have come to recognize as warranting special attention. The formalisation and inclusion of these considerations in the risk assessment procedures is a more recent development (Cowan, 1995). Materials that exhibit the properties of persistence and significant bioaccumulation potential require very careful evaluation prior to any use, however small. PCBs and some pesticides, like DDT and chlordane, are examples of such chemicals. Since surfactants are neither persistent nor bioaccumulative, these aspects are not considered further in this paper.

3. FATE OR EXPOSURE ASSESSMENT TO ESTIMATE THE PEC

The objective of the fate assessment is to estimate the environmental concentration to which organisms will be exposed. To do this, we must consider what compartment the compound enters, whether it will remain in that compartment, whether the compound will be transformed either chemically or biologically and whether the compound will be transported into another compartment. To estimate the environmental concentration in the aquatic environment at tiers 1, 2 and 3, we use the equation:

$$PEC = I\,(1-R)/D \qquad (2)$$

where I is the release concentration and is equal to the influent concentration. This influent concentration is reduced by the removal percentage in wastewater treatment R and the effluent to river dilution factor D.

Tier 1 (Screening Level-I) : In Tier 1, fate assessment, conservative or worst case estimates for usage and removal by wastewater treatment plants are used to calculate PEC. To be conservative, R is set to 0 and D is set to 1 to estimate the aquatic PEC. This assumes that organisms will be exposed to influent concentrations of the compound.

Tier 2 (Screening Level-II) : At Tier 2, data on sorptivity, biodegradability and usage are utilized in a mathematical wastewater treatment plant model (Cowan et al. 1993) to estimate concentrations in wastewater discharged from treatment plants. Conservative (or reasonable, if available) dilution factors are used to estimate the PEC.

Tier 3 (Confirmatory Level) : PEC in Tier 3 are estimated using the same approach as in Tier 2, except that data from laboratory-scale simulation models of real systems (for example, wastewater treatments plants) are used.

Tier 3 (Definitive Level) : Tier 4 is the final tier. In this tier, actual measurement of environmental concentrations and effects on ecosystem structure and function are made. Because concentrations and effects are being measured in actual or realistic systems, an AF of 1 applied to the toxicity data. The most definitive and realistic risk assessment comes from these data.

4. EFFECTS ASSESSMENT TO ESTIMATE THE PNEC

As in the exposure assessment, a tiered approach is used to generate effects data and estimate the PNEC for the compartment of concern. However, we currently believe there is no need to use site specific toxicity data to generate a site specific PNEC as the data do not support geographic differences in species or ecosystem sensitivity. In determining if a bioaccumulation assessment is needed and in evaluating toxicity data, especially in tiers 1 and 2, the hydrophobicity of the compounds being examined must be considered. Typically, as the octanol water partition coefficient (Kow) of a compound increases, the potential for food chain transfer increases and the time to steady state body burdens to be achieved during exposure increases (Connell and Markwell, 1992).

The exposure duration needed for an organism to achieve maximal body burden also increases with hydrophobicity. Hence, toxicity tests may not have been of sufficient duration to allow for full expression of effects during the test and the extrapolation from the available toxicity data to the PNEC may be uncertain. To generate a PNEC from toxicity data within a tier, assessment factors are used to extrapolate available toxicity data to concentrations that protect the ecosystem (Table 2). These factors take into account uncertainties in predicting safe concentrations for a wide variety of species in the environment from laboratory toxicity data on one or a few species.

Tier 1 (Screening Level-I) : In Tier 1 effects assessment, only toxicity information is available, for example, from a *Quantitative Structure Activity Relationship* (**QSAR**) or analogy with related materials or only a single measured acute toxicity value. Since this data provides an acute toxicity estimate with high uncertainty and we are interested in estimating the chronic "safe" concentration in the environment, we divide the effects estimate at Tier 1 by AF of 1000 to estimate PNEC (Table 2).

Tier 2 (Screening Level-II) : At Tier 2, the effects assessment involves measurement of acute toxicity to several species. Typically, an AF of 100 is applied to the lowest acute toxicity value (LC_{50}) to generate PNEC. The reduction in the assessment or safety factor from tier 1 to tier 2 represents our increased confidence in estimating the PNEC from this improved data set.
Tier 3 (Confirmatory Level) : The effects assessment in Tier 3 uses chronic, instead of acute, toxicity data. An AF of 10 is applied to the chronic *No Observed Effect Concentration* (**NOEC**) to determine PNEC. Chronic toxicity data developed from the most sensitive species tested at tier 2 are used to estimate the PNEC.

Tier 4 (Definitive Level) : At Tier 4, a field study would be conducted and NOEC determined from this study used as ecosystem PNEC (Table 2). Tier 4 data are the most realistic but also the costliest.

From this, it can be seen that initial estimates of PNEC and PEC are of a screening nature, and they must be appropriately conservative. As the assessment progresses, more comprehensive data are gathered which better reflect the real world, but are also more costly and time consuming to collect. In some cases, for substances used in high volumes, the assessment may need to proceed to the level of field testing for possible effects and validation of actual environmental concentrations (Tier 4). However, these data are extremely expensive and time consuming to gather and such studies are only conducted for relatively few substances.

In India, as in may other countries, domestic waste is largely disposed directly to the environment, resulting in localized impacts on the ecosystem. In recognition that there are insufficient resources to construct wastewater treatment plants for all discharges, society decides to accept some level of impact or degradation in certain ecosystems. For these sites, the appropriate assessment endpoints would be evaluated differently from those in a so-called "non-impacted aquatic system" (that is, where there is sufficient treatment before discharge). These endpoints would be to ensure no measurable increase in the level of impacts of degradation of these ecosystems.

It is important to note that the intended use of a substance, particularly in the early tiers of the risk assessment process, may have a risk quotient greater than 1, yet still be judged safe ultimately when the assessment is conducted with higher tier data. P&G experience has shown that the safety of many substances, especially those used in small volumes, can be addressed at the initial screening tiers. Only a relatively few substances used in high volumes or with special properties require proceeding to higher tiers to assess their safety. Therefore, the tiered approach helps to optimize the use of resources and permits efficient assessment of safety.

5. APPLICATION OF ERA FOR SURFACTANT (LAS)

The concepts presented above are illustrated briefly by the risk assessment for Linear Alkylbenzene Sulfonate (LAS) in the aquatic compartment. LAS is a major surfactant used by the detergent industry worldwide. Extensive bodies of both effect and exposure information exist and have been published (Viswanath et al, 1997). Numerous aquatic organisms have been tested in the laboratory. Moreover, several field studies have been conducted to determine effects under conditions representing the real world. In the area of fate, LAS biodegradation and removal have been studies in wastewater treatment systems, receiving waters, groundwater and soil. Finally, several monitoring studies, using analytical methodology specific for LAS, have been conducted and confirm the accuracy of predicted concentrations. As a result, LAS is one of the most studied materials used in consumer products, and its safety can be assessed reliably.

The large usage of LAS and its fate and effects profile have required the assessment to move to Tier 4, the definitive level. A no-effect concentration (NOEC) of 0.35 mg/L has been determined in an experimental stream facility. An assessment factor of 1 is applied to this ecosystem NOEC to determine the Tier 4 PNEC, that is, the PNEC (for a non-impacted receiving water) is 0.35 mg/L. This value compares favorably to chronic NOECs of 0.7-1.1 mg/L for fig, 0.6-4.9 mg/L for invertebrates and calćulated hypothetical water quality criteria for continuous exposure. (according to USEPA procedures) of 0.23 mg/L. (11). Monitoring data (US and Europe) show concentrations in receiving waters below wastewater treatment plant outfalls to be generally less than 0.050 mg/L. Thus, the Tier 4 PEC is 0.050 mg/L. Therefore, Risk Quotient at Tier 4 = 0.050 / 0.35, or approximately 0.1. Consequently, the Tier 4 assessment confirms the safety of LAS.

6. REFERENCES

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