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AN SAB REPORT: IMPROVING THE USE CLUSTER SCORING SYSTEM

RECOMMENDATIONS FOR THE USE CLUSTER SCORING SYSTEM PREPARED BY THE ENVIRONMENTAL ENGINEERING COMMITTEE

September 26, 1995

EPA-SAB-EEC-95-017

Honorable Carol M. Browner
Administrator
U.S. Environmental Protection Agency
401 M Street, S.W.
Washington, D.C. 20460

RE: Review of the Use Cluster Scoring System: A Risk Screening Method for Groups of Commercial Chemicals by Use

Dear Ms. Browner:

At the request of the Office of Pollution Prevention and Toxics (OPPT), a Subcommittee of the Environmental Engineering Committee (EEC) of the Science Advisory Board (SAB) reviewed the Use Cluster Scoring System (UCSS). The Subcommittee began its review at the October 26-28, 1994 EEC meeting, received additional documents during the winter, and completed its review at the June 22-23, 1995 meeting.

Clustering chemicals by intended functions could provide efficient risk screening, as well as improved pollution prevention opportunity identification. The UCSS uses algorithms to score chemicals in each cluster according to health and ecological risks. As a result, priorities can be established to address the problems of these clusters in greater detail.

The scope of this review included a response to the following questions which constituted the Subcommittee's charge:

a) How can the clustering process and the methods used to define the chemicals within a use cluster be improved?

b) Are the data sources proposed for the UCSS appropriate, and are there additional useful ones?

c) Are the proposed data sources appropriate to bin chemicals into high, medium, and low risk categories?

d) Are there other general areas/criteria (e.g., waste generation) that should be included in the UCSS?

e) Is the manner in which chemicals and clusters are scored appropriate; and how can uncertainties within the system algorithms and the data sources be treated?"

The findings and recommendations of the Subcommittee are:

a) The proposed UCSS is an important effort to make screening level risk evaluations without the benefit of a complete risk assessment.

b) The methods used to define chemicals in a use cluster need to be improved. For example, a cursory search by the Subcommittee members uncovered a large number of process chemicals in use that were not included in the screening level risk management case study. Therefore, to ensure that each use cluster is as accurate and complete as possible, the Subcommittee recommends the use of several additional data sources including consultation with trade organizations, individual companies, and other federal agencies. Once all chemicals used in a process are identified, their respective functionality needs to be consistently defined.

c) The inclusion of ecological and health concerns, as well as potential for pollution prevention, is a significant feature of the UCSS. Omission of several important data sources for the ecological and health concerns severely limits the utility of UCSS. It should be noted that ecological effects information is often unavailable for many of the chemicals being evaluated. Information on human health effects relatively more abundant. The data sources should be expanded to include data bases from TSCA, as well as QSAR, ECOSAR, and AQUIRE.

d) The basic elements of the scoring system are logically arranged and rely heavily on surrogate exposure measures such as chemical use volumes, number of workers, and octanol-water partition coefficient. A large value of any one of these parameters results in a high exposure estimate. It appears that chemical use volumes are the primary driver of the scoring system. Such a scoring approach leads to severe under- or over-estimates of potential risks and an inappropriate ranking of clusters. The Subcommittee recommends that partitioning behavior, environmental persistence, release or waste concentrations be given more weight and appropriate level of effort be allocated to generate the databases for the UCSS.

e) The UCSS be expanded to include consideration of the cost and efficacy of substitute chemicals to provide a measure of performance potential. Some cost-benefit analysis needs to be considered for the overall cluster evaluation. This analysis could use a relative weighting factor to provide further guidance for prioritizing clusters for evaluation in greater detail. No specific method for cost-benefit analysis has been recommended by the Subcommittee acknowledging that the Agency will be able to adopt an appropriate method based on its previous experiences.

The Subcommittee appreciates the opportunity to review the scoring system, and we look forward to a written response to its recommendations for improving the UCSS.

Sincerely,

Dr. Genevieve M. Matanoski, Chair
Executive Committee

Dr. Ishwar P. Murarka, Chair
Environmental Engineering Committee

Dr. James H. Johnson Jr., Chair
Use Cluster Scoring System Subcommittee

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ABSTRACT

At the request of the Office of Pollution Prevention and Toxics (OPPT), a Subcommittee of the Environmental Engineering Committee (EEC) of the Science Advisory Board (SAB) reviewed the Use Cluster Scoring System (UCSS) which is being developed by OPPT. The primary purposes for clustering chemicals by intended functional use are to: a) efficiently screen large numbers of commercial chemicals; and b) identify opportunities to prevent pollution within the resulting use clusters. Algorithms are used to score chemicals in each cluster according to their health and ecological risks in order to set priorities for future evaluation of these clusters.

The review focused on: a) improvement of the clustering process; b) validity of the UCSS data sources; c) capability of UCSS to sort chemicals by risk categories; d) other general areas and criteria that could be included in UCSS; and e) the soundness of the system algorithms.

The proposed UCSS is an important initial effort to construct a screening-level risk statement for clusters of chemicals by use. The Subcommittee report suggests ways to enhance that effort.

The primary recommendations are that the Agency should: a) identify and use additional significant data sources for the ecological and health concerns; b) modify the surrogate exposure measures so that the score is not dominated by wide use in industry, but includes the impacts of bioaccummulation, persistence and exposure pathways; c) include measures of performance potential in the chemical-specific analysis; and d) use a cost-benefit analysis for the overall cluster evaluation.

Keywords: chemical use, scoring systems, pollution prevention, ranking, relative risk

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1. EXECUTIVE SUMMARY

At the request of the Office of Pollution Prevention and Toxics (OPPT), a Subcommittee of the Environmental Engineering Committee (EEC) of the Science Advisory Board reviewed the Use Cluster Scoring System (UCSS) being developed by the OPPT. The primary purposes for clustering chemicals by intended functional use are to: (1) efficiently screen large numbers of commercially used chemicals; and (2) identify opportunities to prevent pollution within the use clusters. Algorithms are used to score chemicals in each cluster according to their health and ecological risks in order to set priorities for the evaluation of clusters in greater detail. To make this effort even more useful, the Subcommittee made several observations and recommendations including:

a) The proposed UCSS is an important effort to methodically use existing information to make a screening-level risk statement about clusters of chemicals by use.

b) The inclusion of ecological and health concerns as well as potential for pollution prevention in the UCSS is a significant feature. However, the UCSS, as well as its use in the screening-level Risk Management (RM-1) dossiers, do not take advantage of several important data sources for the ecological and health concerns. This omission severely limits the utility of UCSS. It should be also noted that ecological effects information is often unavailable for many of the chemicals being evaluated. Information on human health effects is relatively more abundant.

In addition, the formation of clusters in the RM-1 dossiers were not well delineated on the basis of functionality and substitutability as required by the UCSS. Therefore, to ensure that each use cluster is as accurate and as complete as possible, the Subcommittee recommends the use of several additional sources including consulation with trade organizations, individual companies and other federal agencies.

c) The Subcommittee noted with concern that the exposure component of the algorithm by means of surrogate exposure measures (e.g., chemical use volume and octanol-water partition coefficient) drives the scores for clusters. As a result, if a chemical is widely used in the industry, it could receive a high ranking for human and ecosystem exposure, regardless of its tendency to bioaccumulate, its tendency to persist in the environment, or its potential exposure pathways and concentrations of environmental releases. This limitation is judged to be a serious flaw that must be remedied prior to the application of the UCSS.

d) The Subcommittee recommends that some measure of performance potential be included in the chemical-specific analysis. The performance potential should consider factors such as the cost and efficacy of the substitute. A cost-benefit analysis needs to be considered for the overall cluster evaluation. This analysis could use a relative weighting factor to compare different clusters and provide further guidance for prioritizing clusters to be evaluated in more detail. No specific method for cost-benefit analysis has been recommended by the Subcommittee acknowledging that the Agency will be able to adopt an appropriate method based on its previous experiences.

2. INTRODUCTION

At the request of the Office of Pollution Prevention and Toxics (OPPT), a Subcommittee of the Environmental Engineering Committee (EEC) of the Science Advisory Board (SAB) reviewed the Chemical Use Cluster Scoring Methodology (September 30, 1994 - draft) under development by the OPPT. The scientific and technical aspects of this methodology, termed the Use Cluster Scoring System (UCSS), were reviewed on October 27, 1994, in light of its intended uses. To aid in the evaluation, two pilot studies on the use of UCSS for First-Level Risk Management (RM-1) were provided to EEC. The studies were entitled "Corrosion Inhibitors Used in Industrial Boilers" and "Positive Photoresist Developers for Semiconductors." The appropriateness of the use of UCSS for these RM-1 assessments is included in the review.

OPPT's primary purposes in clustering chemicals around intended functional use are to: a) efficiently screen large numbers of commercial chemicals by risk factors; and b) identify pollution prevention opportunities within the resulting use clusters. By applying algorithms to score chemicals in each cluster on the basis of health and ecological risks, clusters can then be prioritized for further evaluation.

OPPT requested particular consideration by the Subcommittee to the following aspects of the use cluster methodology:

a) How can the clustering process and the methods used to define the chemicals within a use cluster be improved?

b) Are the data sources proposed for the UCSS appropriate, and are there additional useful ones?

c) Are the proposed data sources appropriate to bin chemicals into high, medium, and low risk categories?

d) Are there other general areas/criteria (e.g., waste generation) that should be included in the UCSS?

e) Is the manner in which chemicals and clusters are scored appropriate; and how can uncertainties within the system algorithms and the data sources be treated?

3. FINDINGS AND RECOMMENDATIONS

The Subcommittee recognizes that a complete risk assessment on every chemical is not practical. Therefore, a rank ordering of groups of chemicals could enable the EPA and industry to identify the best candidates for reduction and replacement in a pollution prevention program on the basis of potential for adverse health and ecological effects. Accordingly, the UCSS is a method of selectively assessing the impacts of a chemical within a designated use area, thereby somewhat simplifying the exposure assessment. An excellent review of chemical use clustering methods is provided by Davis et al. (1993). The Subcommittee notes and concurs with the inclusion of ecological impacts with health concerns and potential for pollution prevention.

The following suggestions to enhance the scientific merit and usefulness of the scoring system are presented in response to the questions posed in the Subcommittee's charge.

3.1 How Can the Clustering Process and the Methods Used to Define the Chemicals Within a Use Cluster be Improved?

The Subcommittee recommends improvement in two specific areas, i.e., the methods used to define chemicals in a cluster, and the functionality and substitutability of chemicals in a cluster. The methods used to define chemicals within use clusters are deemed inadequate. For example, in the First-Level Risk Management (RM-1) case study for boiler water treatment processes, a cursory search of the literature by Subcommittee members uncovered a number of process chemicals in use that were not included in the analysis. Moreover, several of the higher scoring chemicals which were included in the corrosion inhibitor cluster may actually not be used as corrosion inhibitors in industrial boilers. Therefore, to ensure that each use cluster is as accurate and as complete as possible, the Subcommittee recommends the use of several other data sources, such as:

a) Trade associations for each use area who could poll their membership with regard to chemical use. The EPA Design for Environment program is an example of where this approach has been used effectively.

b) Industries that produce and supply alternative chemicals. For example, EPA, Research Triangle Park, North Carolina has held several workshops on low- and no-VOC coatings with these groups in attendance. The National Roundtable of Pollution Prevention Programs currently is documenting these workshops.

c) DOD and DOE who currently have alternative chemical initiatives, such as with personnel at Wright-Patterson AFB and Idaho Falls National Laboratory,

respectively.

After identifying the chemicals used in a particular industrial process, their respective functionality needs to be defined. In the RM-1 for semiconductors, several forms of functionality are listed , e.g., photoresists, developers, buffers and surfactants, and other wetting agents. However, the table of chemicals for the use cluster does not designate the chemicals by functionality which is important because substitutes can only be identified within a listing of chemicals by using functionality. Hence, the utility of the UCSS in this RM-1 is not apparent.

In contrast, in the RM-1 for "Corrosion Inhibitors Used in Industrial Boilers," an attempt was made to assign the component chemicals of a formulation to a use cluster on the basis of their function in the formulation. In most cases, classifying them by their function in a formulation will be very difficult and may result in chemicals being misclassified. In addition, components in formulations frequently function synergistically and their real function is often not apparent.

A second issue for each use cluster is the assumption that chemicals in a use cluster can substitute for each other without the loss of effectiveness. This assumption is not valid in the RM-1, “Analysis for the Corrosion Inhibitors Used in Industrial Boilers.” In this RM-1, the effectiveness of chemicals in the clusters is not equal and, in most cases, the chemicals also are not substitutable (See Appendix A).

3.2 Are the Data Sources Proposed for the UCSS Appropriate, and Are There Additional Useful Ones?

Several of the data sources are considered incomplete and the uses inappropriate. The Subcommittee recognizes that screening for priority setting needs to address large numbers of substances with maximum use of available data. However, data quality and relevance need to be assured, since the inclusion of inappropriate and spurious data will lessen the overall accuracy and usefulness of the scoring system. Hence, the effort could be strengthened by considering other data bases such as:

a) TSCA information on chemicals solicited from chemical suppliers;

b) Stanford Research Institute databases on chemicals and their industrial use;

c) information solicited directly from industries; and

d) information solicited from professional and trade associations, e.g., the American Chemical Society.

The Subcommittee also noted a relative dearth of data sources for ecological data elements in the UCSS. Therefore, it was very difficult to judge this aspect of the results and utility of the current approach. In that respect, Table 1 developed based upon the experience of Subcommittee members, provides a qualitative assessment of the ecological effects data elements currently utilized by the UCSS. A review of how other scoring procedures incorporate ecological data could lead to the adoption of a better approach that would significantly improve the section on the potential for ecological effects.

Table 1. Assessment of Ecological Data Elements in UCSS

Element	Assessment
AWQC, acute and chronic	Very limited use because so few exist
RQ for aquatics	Not a very reliable source of direct toxicity
QSAR	Good, if used properly
SATeam	Acceptable as a last resort
Chemical EcoEstimate	No reason to consider

With respect to the currently used data elements in the UCSS, reliable and high-quality measured acute toxicity data sources are readily available for every chemical. These include QSAR (Environmental Estimator and Modeling), ECOSAR, AQUIRE (Aquatic Information Retrieval) and HSDR (Hazardous Substance Data Bank). Appendix B summarizes the information available in these sources, and Appendix C provides additional sources on predictive environmental fate properties and toxicity and environmental fate data sources. Chronic NOEC (no observable effect concentration) measured data are available through literature searches for some of the chemicals. NOECs also can be obtained using established acute-to-chronic ratios.

Other important peer-reviewed data bases which could be cited include EPA's Drinking Water Standards, Threshold Limit Values (TLV) of the ACGIH, and Permissible Exposure Limits (PEL) of OSHA. Although the TLVs and the PELs are designed for the protection of workers during a 40-hour work week for a working lifetime, they can be used to estimate values approximating RfCs (Reference Concentrations) by the application of time-weighted averaging (Haber's Rule), and the application of a safety factor of ten to account for the greater variability of the general population when compared to workers. In application, this results in the following:

$$\text{Pseudo RfC} = \text{TLV} \times 0.1 \times \frac{8}{24} \times \frac{5}{7} = \text{TLV} \times 0.024$$

The components of the exposure portion of the algorithm have only remote relationships to exposures. It is uncertain that the exposure portion of the algorithm will allow the construction of even an approximate view of the chemical constituents within clusters. Consequently, it also will be virtually impossible to estimate relationships among clusters. The exposure potential elements of persistence, bioconcentration, and some estimate of volume used/released are appropriate to include in the UCSS. However, there is a need to enhance the extent of the data base for bioconcentration and persistence. The Subcommittee suggests that other published procedures be reviewed to select options to derive estimates and highlight reasonable approaches to estimate bioconcentration and persistence parameters. Sources to consider include the following:

a) The European Community scoring procedure (Van der Zandt and Van Leeuwen, 1992) provides a useful model for a more sophisticated procedure which carries exposure estimates to environmental media concentrations. Effects data are then compared to exposure concentrations, and potential adverse effects evaluated via the margin of safety.

b) The University of Tennessee Chemical Ranking System (Davis et al., 1993) offers the advantage of a minimum data base requirement with reliance on QSAR to fill data gaps.

c) In February 1995, the Society for Environmental Toxicology and Chemistry held a workshop on Ranking and Scoring Methodologies which resolved some of the issues identified in the UCSS. Agency personnel should review the outputs of this important workshop when published.

3.3 Are the Proposed Data Sources Appropriate to Bin Chemicals Into High, Medium and Low Risk Categories?

The Subcommittee considered the advantages and disadvantages of relying upon a high, medium, and low categories approach. With the frequent use of high, medium, and low value judgments, the model has the appearance of being subjective rather than objective. In many instances, value judgments are made by arbitrarily dividing numerical data into these three groups. The rationale for these groupings is not apparent, and ignores a great deal of information that is very useful in understanding why one chemical might be better or worse for the environment.

The Subcommittee suggests that consideration be given to eliminating the high, medium, and low categories in favor of rank ordering the raw data. Chemicals could then be ranked on the basis of each characteristic. The rank orders for each characteristic for any one compound could then be combined to develop a numeric score for an individual compound as is currently done, e.g., chemicals could be ranked by Use Volume. The chemical with the highest Use Volume could be assigned a value of 1, while that with the lowest, a much higher number. This approach is expected to provide a more meaningful relative ranking of the impact of chemical use on the environment.

3.4 Are There Other General Areas/Criteria (e.g., waste generation) That Should Be Included in the UCSS?

The Subcommittee recommends several enhancements to improve the scoring of chemicals and clusters. These include more appropriate data sources for the exposure side of the scoring algorithm, a measure of performance potential of chemicals, use of high quality, consistent data sources for ecological and health risks, consideration of pollution prevention alternatives, and use of a credibility check to ascertain reasonableness of UCSS outputs.

Potential for pollution prevention, e.g., recycling, should also be included in the screening evaluation. Trade organizations could be consulted at the UCSS stage, informed of the cluster(s) being examined, and asked if any new emerging technologies are being evaluated which have the potential for major source reduction.

3.5 Is the Manner in Which Chemicals and Clusters are Scored Appropriate; and How Can Uncertainties Within the System Algorithms and the Data Sources be Treated?

The basic elements of the Chemical Use Clusters Scoring System (UCSS) are illustrated in Figure 1. The system currently considers four elements: a) Human Risk Potential, b) Ecological Risk Potential, c) EPA Interest, and d) Cluster Pollution Prevention Potential. The system scores both the Human and Ecological Risk Potentials three times higher than the latter two, i.e., EPA Interest and the Pollution Prevention Potential. The Subcommittee recommends the inclusion of an additional screening element to provide a measure of chemical performance.

3.6 Additional Comments

While the basic elements of the UCSS algorithm are logically arranged, the Subcommittee recommends several enhancements to improve the scoring of chemicals and clusters. These include: incorporation of additional data for the exposure portion of the scoring algorithm, a measure of performance potential of chemicals, use of high quality, consistent data sources for ecological and health risks, consideration of pollution prevention alternatives, and use of a credibility check to ascertain reasonableness of UCSS outputs. The following enhancements in the scoring algorithm have the potential to improve the ultimate application of the UCSS.

Figure 1. Schematic Diagram of Chemical Use Clusters Scoring Algorithm (Source: U.S. EPA, 1993)

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(Later add electronically)

a) As designed and implemented, the cluster scoring system heavily weights exposure data. A qualitative exposure ranking of high, medium, or low weighs both human hazard and ecological hazard information. Unfortunately, there are no easily accessible data on exposure. In place of exposure pathway and exposure level (concentration) information, the cluster scoring system employs surrogate exposure measures, which include chemical use volumes, number of workers, and octanol-water partition coefficient. A large value of any one of these parameters results in a high-exposure estimate. For example, if a chemical is used widely in the industry, it could receive a high ranking for human and ecosystem exposure, regardless of its tendency to bioaccumulate, its tendency to persist in the environment, or the potential pathways and concentrations of environmental releases.

It appears that chemical use volumes are the primary drivers of the scoring system. Such a scoring approach may lead to severe under- or over-estimates of potential risk and an inappropriate ranking of clusters. It is recommended that partitioning behavior, environmental persistence, release or waste system concentrations be given more weight in the exposure estimation scoring process, and a major effort be employed to improve the data bases in these areas.

Also, care should be used in determining what information should be entered into the model. Parameters that are functionally related to one another should not be included in the model. For example, "Reportable Quantities" were likely developed on the basis of "Reference Doses" or some other toxicological parameter. The base parameter should be used in favor of the derived parameter.

b) Some measure of performance potential, i.e., the effectiveness of a substitute, should be included in the chemical-specific analysis. Figure 2 shows a suggested screening algorithm. The performance potential measure could consider factors such as cost of substitution and efficacy of substitute, if these data are available. If not, end-user opinion could be solicited to establish a relative score.

In addition, some type of cost/benefit analysis should be considered for the overall cluster evaluation (See Figure 2). This analysis could be used as a relative weighting factor to compare the different clusters and provide further information for identifying clusters to be evaluated in more detail. No specific approach or methodology is suggested.

c) Cluster scoring for ecological effects is appropriate when the data are available to fill in the matrix. Uncertainty of data in a procedure designed for screening purposes can be handled adequately with some general expression of quality. For

aquatic toxicity data, actual tests are of higher quality than QSAR-derived data. When QSAR data are used, its use should follow the current accepted practices.

d) The evaluation of human health hazards for specific chemicals is probably the strongest segment of the UCSS. However, the current procedure for health hazard scoring contains a number of inconsistencies. The Subcommittee concurs that Reference Dose (RfD) and Reference Concentration (RfC) values are generally of high quality and have undergone internal review by EPA, but often have not benefited from formal external peer review. The present methodology shows an inconsistent and unsupportable set of relationships in scoring thresholds between RfD and RfC values. As an alternative, equivalent exposures can be approximated by assuming that an adult consumes 2 liters of water per day, inhales 20 m^3 of air, and weighs70 kg. Under such conditions a daily dose of 0.001 mg/kg of body weight would correspond to a dose of 0.07 mg/20m^3 or 0.0035mg/m^3 of air inhaled, or 0.035 mg/L of water consumed.

Reportable Quantities (RQ) and Threshold Planning Quantities (TPQ) are values that are derived through their own methodologies. Their construct usually considers a variety of potential effects, including flammability, explosivity, toxicity, and other conditions. When they are based upon toxicity alone, they also incorporate severity of responses and their own scaling factors. Consequently, the reportable quantity has become more of an administrative device and is no longer a translatable descriptor of toxicity. Although these RQ and TPQ values have received some peer review, it was for a different purpose.

Figure 2. Schematic Diagram of Recommended Changes to the Chemical Use Clusters Scoring Algorithm (Modified from: U.S. EPA, 1993)

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Table 9 of Reference 1 cites a number of instances of using NOAEL and LOAEL values. The ratios of the associated scoring thresholds suggest that, in fact, these were used to calculate values equivalent to RfDs, using the usually accepted uncertainty factors. Methodologies also exist to estimate NOEC or NOAEL values from more acute toxicological data, albeit with increasing uncertainty. Major data bases that can assist in these endeavors are the Registry of Toxic Effects of Chemical Substances (RTECS) by NIOSH, the Hazardous Substance Data Base by the National Library of Medicine, and Toxline. The units of measurements for these data can be made equivalent in terms of dose in mg/kg-day, or their equivalent water or air concentrations. Thus, it will be possible to enter the dose rate directly into the scoring algorithm.

The RfC, RfD and derived limiting values relate to dose rates that must be exceeded by some amount before an effect may be expected. Thus, arranging the RfDs or their equivalents from lower to higher doses creates an ordinal grouping from highest to lowest toxicity potential.

The careful distinction between RfC and RfD values also indicates one of the differences between exposure media. The contaminant releases and/or their subsequent fate and transport are often media specific, so that it may be desirable to differentiate between potential exposures through air and water (consider the use of Henry's constant or McKay's modeling approaches). This can also have many benefits for the assessment of ecological effects.

The data quality will vary as more and more steps are entered in the derivations of the RfDs or their equivalents. It is desirable to carry an index of uncertainty along with the individual estimates.

e) The current model does not address the “no” chemical alternative which exists for many of the use categories. Information on this alternative can be obtained from industry trade associations, the National Roundtable for Pollution Prevention members, and the Office of Pollution Prevention of EPA. These alternatives should be identified and listed on the cluster for each use. The Subcommittee recognizes that substitutes are not always the best means for pollution prevention, and often only shift or delay the problems. Generally, there are no drop-in substitutes, and often the substitutes may cause other problems, for example, trading a human health exposure for an aquatic toxicity problem.

f) A reality check must be conducted on the model output to assure that it is reasonable and thus credible. The Subcommittee recommends the use of external panels inclusive of affected industries, to judge merits of rank ordering outcomes from the cluster scoring.

The Subcommittee was not able to ascertain reliability of the data and impacts on the UCSS output, and therefore, proposes the application of the following as a means to determine the order of magnitude of the variability of the data. If the values are ± 30 percent or so, the Pareto Principle (80/20 Rule) will negate the uncertainty, i.e., 20% of the chemicals will cause 80% of the problems (see, for example, Ishikawa, 1968). Rank ordering of the major impact chemicals will not be changed by the uncertainty in the data with the ± 30 percent level. Even at the +100 percent level, the impact will not be overriding. The work group should consult the literature on the use of Pareto Analysis for rank ordering.

As a final point, the Subcommittee recommends that coordination of the UCSS with other scoring activities within the Agency be undertaken.

REFERENCES CITED

Davis, G.A., et al., 1993. Chemical Ranking for Potential Health and Environmental Impacts, University of Tennessee, Center for Clean Products and Clean Technologies, Knoxville, TN.

Ishikawa, K., 1968.Guide to Quality Control, Quality Resources Publishing Co., White Plains,NY 1968

Van de Zandt, D.T.J. and C.J. Van Leeuwen, 1992. A Proposal for Priority Setting of Existing Chemical Substances. Netherlands Ministry of Housing, Physical Planning and the Environment, Risk Assessment and Environmental Quality Division.

DOCUMENTS REVIEWED

EPA, 1994. Chemical Use Clusters Scoring Methodology (Draft), September, 1994, Chemical Engineering Branch, Office of Pollution Prevention and Toxics, U.S. Environmental Protection Agency, Washington, DC.

EPA, 1994. RM-1 Use Cluster Dossier: Corrosion Inhibitors Used in Industrial Boiler (Draft Report) September 1994,, Office of Pollution Prevention and Toxics, U.S. Environmental Protection Agency, Washington, DC.

EPA, 1994. RM-1 Use Cluster Dossier: Positive Photoresist Developers for Semiconductors, August, 1994. Office of Pollution Prevention and Toxics, U.S. Environmental Protection Agency, Washington, DC.

ACRONYMS

AQUIRE:	a data base focused on the toxic effects of chemical substances on freshwater and salt-water organisms (excluding aquatic mammals, birds, and bacteria)
ECOSAR:	a computer program for estimating the ecotoxicity of industrial chemicals based on structure activity relationships (SARs)
EEC:	Environmental Engineering Committee, Science Advisory Board, U.S. EPA
HSDB:	Hazardous Substance Data Base by the National Library of Medicine, a factual, non-bibliographic database containing information concerning toxicological and environmental effects of approximately 4300 chemicals
LOAEL:	Lowest observable adverse effect level
NOEC:	No Observable Effect Concentration
NOAEL:	No Observable Adverse Effect Level
OPPE:	Office of Policy, Planning and Evaluation, U.S. EPA
PEL:	Permissible Exposure Limits (PEL) of OSHA designed for the protection of workers during a 40-hour work week for a working lifetime
QSAR:	an on-line chemical property system that uses Quantitative Structural Activity Relationship methods
RfC:	Reference Concentrations
RfD:	Reference Doses
RM-1:	First-Level Risk Management assessment
RQ:	Reportable Quantities
RTECS:	NIOSH's Registry of Toxic Effects of Chemical Substances, a major data base
SAB:	Science Advisory Board, U.S. EPA
SETAC:	Society for Environmental Toxicology and Chemistry
TLV:	ACGIH Threshold Limit Values designed for the protection of workers during a 40-hour work week for a working lifetime
TPQ:	Threshold Planning Quantities
TSCA:	Toxic Substances Control Act
UCSS:	Use Cluster Scoring System

APPENDIX A

SUBCOMMITTEE REVIEW OF

RM-1 -- USE CLUSTER DOSSIER: CORROSION INHIBITORS USED IN INDUSTRIAL BOILERS DECEMBER 5, 1994 DRAFT REPORT

The following review of the draft RM-1 dossier on Corrosion Inhibitors Used in Industrial Boilers was conducted to assist in the SAB review of the UCSS and its implementation into RM-1. The comments provided in the review should be used to improve the RM-1, and to reinforce the recommendations made in the main body of this report for improving the overall usefulness of the UCSS.

Review of the RM-1 dossier uncovered several major areas of concern with corresponding opportunities for improvement. The identified areas of concern that will be discussed in the review are as follows:

1. Cluster Chemical Selection/Identification
2. Chemical Volume/Exposure Data
3. Process Regulatory Trends

<u>Cluster Chemical Selection/Identification</u>

The most serious concern identified in the review of the corrosion inhibitor is the selection of chemicals defining the use cluster. The Subcommittee is concerned that several of the chemicals included in the use cluster are not used as corrosion inhibitors in industrial boilers. Two chemicals of primary concern with respect to this issue are arsenic and antimony.

Several experts in the field of industrial boiler water treatment were consulted to verify the use of arsenic and antimony in industrial boilers. An attempt was made to verify the use of these chemicals by consulting the original reference cited in the RM-1 [Kirk-Othmer. 1991. Corrosion and Corrosion Control (Vol. 7), Steam (Vol 21). Kirk-Othmer Encyclopedia of Chemical Technology. 3rd and 4th Editions. New York, NY: John Wiley and Sons.] Although listed as corrosion inhibitors which have been used in aqueous systems, neither arsenic nor antimony could be confirmed for cluster use (Kirk-Othmer, 3rd and 4th Editions). A number of other cluster chemicals including chromate, sulfur dioxide and benzotriazole are also questionable as to their use in industrial boilers.

As discussed in the Draft Corrosion Inhibitor Dossier [Submitted by Versar, Inc. 1994 to the Risk Analysis Branch, Office of Pollution Prevention and Toxics, U.S. Environmental Protection Agency] arsenic and antimony ranked high for human health concerns, with antimony also high for ecological concern. If these chemicals were not included in the use cluster, it is possible that the corrosion inhibitor cluster would not have scored sufficiently high to warrant a RM-1 screening level assessment. The possibility of including chemicals not representative of a use cluster presents a potentially serious flaw to the UCSS and points out the need to include trade organizations and other outside expert advice in the UCSS process.

Volume/Exposure Data

The UCSS methodology is judged to be inappropriately weighted with respect to volume and exposure data which drive the scoring of clusters. To compound further, the data generally are of high uncertainty. Table 6 of the dossier summarizes the corrosion inhibitor exposure data. Limitations in the quality and accuracy of the data are recognized and discussed in the draft RM-1 in Section 7.2. A case in point illustrating the limitations of the data is the use volume estimate of 2,300,000 lbs in Table 6 for hydrazine (although the use is on a volume basis, the actual quantities are given in weight). Hydrazine is typically applied at part per billion (ppb) levels as a boiler water oxygen scavenger and is primarily used only in high pressure boilers found mostly in the power generation industry. Hydrazine use in industrial boilers is limited (41 sites per Table 6), and suspected to be much less than 2,300,000 lbs. Other data entries in Table 6 which are suspect include the use volume estimate for arsenic (2.25 million lbs), the use volume estimate for ethylenediamine (1.93 million lbs) and the number of sites estimate for cyclohexylamine (107, considered low).

As presented in the UCSS review, several recommendations are made for improving the quality of the use volume/exposure data, and for reducing the significance of these data in driving the UCSS methodology.

Process Regulatory Trends

In a number of sections of the draft RM-1, references and parallels are drawn to regulatory actions, pollution and process trends in industrial cooling water treatment. The Subcommittee recommends that caution be used in making these comparisons, and that attention be given to the fact that the technology used for boilers varies with the use of the boiler (Kirk-Othmer, 3rd Edition). Comments and suggestions with respect to specific sections of the draft RM-1 which discuss trends are as follows:

a) *Section 4.3, page 7*

The trends discussed with respect to new inhibitors to replace chromium compounds pertains to cooling water corrosion control. Parallels to boiler water are overstated.

b) *Section 5.0, page 9*

Corrosion inhibitors (e.g., phosphate and zinc) are added to once-through cooling water. The relevance of the last three paragraphs in Section 5 to boiler water treatment is not clear and should be restated.

APPENDIX B

Ecotoxicity Data Sources

Name: QSAR - Environmental Estimation and Modeling
Source: TDS Numerica™
Producer: Hunter Systems and the IPA at Montana State University
Summary of Content: QSAR is an on-line chemical property evaluation system that uses Quantitative Structural Activity Relationships methods. This system is a tool for estimating chemical properties and predicting environmental fate, persistence, and the transport of chemical substances in the environment. Calculations are based on the chemical structure and property values stored in the data base or entered by the user. Properties estimated include log P, water solubility, pKa, bioconcentration factor, soil adsorption and vapor pressure. Environmental partitioning and aquatic toxicity estimates are also provided. Compounds are identified by CAS number or SMILES notation.

Name: ECOSAR
Source: National Technical Information Service (NTIS), Item Number PB94-500485
Producer: USEPA, Office of Pollution Prevention, and Toxics, February, 1994

Summary of Content: ECOSAR is a computer program for estimating the ecotoxicity of industrial chemicals based on structure activity relationships (SARs). Originally developed to estimate the aquatic toxicity of chemicals reviewed by the USEPA in response to Pre-Manufacture Notices mandated by Section 5 of the Toxic Substance Control Act, such estimations have been found to have a wide use in hazard assessment, ecological risk assessments, and general aquatic toxicology.

Name: AQUIRE (Aquatic Information Retrieval)
Sources: Chemical Information Systems; TDS Numerica™
Producer: USEPA Environmental Research Laboratory, Duluth, MN (ERL-D) - sponsored by the Office of Toxic Substances of the USEPA

Summary of Content: The AQUIRE database focuses on the toxic effects of chemical substances on freshwater and saltwater organisms (excluding aquatic mammals, birds, and bacteria). Data types include acute and chronic toxicity, bioaccumulation, and sub-lethal effects. Fathead minnow toxicity data generated by the EPA Duluth laboratory is included.

Name: HSDB (Hazardous Substance Data Bank)
Sources: STN International (private); TOXNET (public)
Producer: Toxicology Information Program of the National Library of Medicine

Summary of Content: The Hazardous Substance Data Bank (HSDB) is a factual, non-bibliographic database containing information concerning toxicological and environmental effects of approximately 4300 chemicals. Data regarding environmental impact, human exposure, detection methods, manufacturing and use information, and emergency handling procedures may also be available. Some aquatic toxicity data is available in the “Wildlife Toxicity:” field. This data base contains narrative descriptions of environmental fate and impact. The data sources are identified. This database is updated quarterly.

APPENDIX C

PREDICTIVE PROGRAMS FOR PHYSICAL AND ENVIRONMENTAL FATE PROPERTIES

ECDIN (Environmental Chemicals Data & Information Network)

Source: TDS Numerica™

Producer: Environmental Research Programme of the Joint Research Centre of the Commission of the European Communities

This system contains important experimental and regulatory information from the U.S., Canada, Eastern and Western Europe and the Pacific Rim. Over 25,000 chemicals are included, with data including chronic and acute toxicity, concentration and fate in the environmental, physical and chemical properties. In addition, legislation and rules, occupational safety and health, and detection methods are available.

ENVIROFATE (Environmental Fate and Physical Property Database)

Source: Chemical Information Systems

Producer: Office of Toxic Substances of the U.S. EPA/Syracuse Research Corporation (SRC)

ENVIROFATE includes data on environmental transformation rates (biodegradation, oxidation, hydrolysis, photolysis) and physical-chemical properties (water solubility, log partition coefficient, vapor pressure). Bioconcentration data is also available. Most of the data in ENVIROFATE is also present in the Environmental Fate Database.

Environmental Fate Database (Components: **CHEMFATE, BIODEG, BIOLOG, DATALOG)**

Source: TDS Numerica™

Producer: Syracuse Research Corporation

CHEMFATE contains experimental data regarding chemical properties, environmental transport properties, octanol/water partition coefficients, degradation studies, and field monitoring covering more than 1200 chemicals.

BIODEG contains experimental biodegradation data for more than 800 substances. Full reference information is provided.

BIOLOG and DATALOG contain bibliographic references covering biodegradation data (for more than 12,000 chemicals) and environmental fate data (for more than 15,000 chemicals), respectively. References for BIODEG and CHEMFATE are included in these systems, along with additional sources of data.

Log P and Related Parameters Database

Source: TDS Numerica™

Producer: Medicinal Chemistry Project at Pomona College

The Log P and Related Parameters Database provides experimentally determined partition coefficients (Log P) for 14,000 organic compounds using more than 300 solvent pairs including octanol/water (Low Kow), the standard for this system. Acid dissolution constants (pKa), references, comments, and evaluations by the database authors, and a large compilation of related parameters also can be retrieved. Log P values are used in environmental analysis and in models that predict biological activity.

OHM/TADS (Oil and Hazardous Materials/Technical Assistance Data System)

Source: Chemical Information Systems, Inc.

Producer: Superfund Program of the U.S. Environmental Protection Agency

OHM/TADS provides access to a data file created to aid emergency response teams in the retrieval of chemical-specific response information. Types of information include reactivity information, detection information, chemical and physical properties, environmental fate and chemical data, toxicological data, and hazard information. The system was last updated in 1985, and contains records for 1,482 substances.

ISHOW (Information System for Hazardous Organics in Water)

Source: Chemical Information Systems, Inc.

Producer: Office of Toxic Substances of the U.S. Environmental Protection Agency

The ISHOW system covers six types of physical property data: melting point, boiling point, vapor pressure, water solubility, log partition coefficient (Log P) and dissertation constants. Bibliographic references are included. Approximately 5,400 chemicals (16,600 records) were included as of December, 1992. ISHOW was last updated in 1985, and no further updates are anticipated.

APPENDIX D

DATABASE SOURCES

National Technical Information System
5285 Port Royal Road
Springfield, VA 22161

(703) 487-4650

Chemical Information Systems, Inc.
A Division of PSI International, Inc.
810 Gleneagels Court, Suite 300
Baltimore, MD 21286

(800) 247-8737
(410) 196-0712

TDS Numerica™
Technical Database Services, Inc.
135 West 50th Street, Suite 1170
New York, NY 10020-1170

(212) 245-0044

STN International
c/o Chemical Abstracts Service
P.O. Box 3012
Columbus, OH 43210

(614) 447-3600

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