**PEER REVIEW OF EPA'S HAZARDOUS WASTE
IDENTIFICATION RULE RISK ASSESSMENT MODEL**

Physical/Chemical Properties of HWIR Chemicals

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NOTE

This report was compiled by Eastern Research Group, Inc. (ERG), an EPA contractor, under Contract Number 68-W-99-001. The report presents comments provided by peer reviewers on the *Physical/Chemical Properties of HWIR Chemicals* document that is part of EPA's Hazardous Waste Identification Rule risk assessments. The actual reviewer was performed in 1998 under Contract Number 68-W5-0057.

The comments presented in this report have been compiled by topic and by individual peer reviewer. As EPA requested, this report provides the peer review comments exactly as they were submitted to ERG. Also attached are the original comments submitted by each individual reviewer.

HWIR98 Research Plan

CHEMICAL and BIOLOGICAL FATE DATA TEAM

Background

The chemical and biological fate data team was charged with developing the chemical-specific date required for the HWIR-base exposure and risk assessment. Within the HWIR exposure and risk assessment there exists a wide range of environmental settings (i.e., combinations of physical/biological/ chemical conditions) within which chemicals of concern are disposed, transported, and transformed. Examples of physically based environmental settings would include each of the major environmental media (i.e., atmosphere, surface water, groundwater, vadose zone, surface soils, aquatic sediments, and biota). Within these physical settings there exists a wide range of environmental conditions (i.e., soil and sediment type, microbial activity, redox zonation, etc). The overall objective of this effort is to understand the fate data needs (i.e., kinetic and thermodynamic constants) of the HWIR assessment and provide the science-based data via referenced literature values, predictive chemical modeling, and/or expert judgement.

The HWIR assessment can be viewed as a tracking of individual chemicals from specific waste streams disposed of in a waste management unit (e.g., landfill, waste pile, surface impoundment, land application unit), into the surrounding multimedia environment via various natural release processes (e.g., volatilization, leaching, runoff, erosion) and through the multimedia environment to locations where human and ecological receptors are likely to contact the chemical. Environmental simulation models which require certain chemical- secific data are used to perform this tracking and characterize the resulting exposure and risks.

It is recognized that all of the data needs can not be satisfied with the measured values, the environmental conditions within which the contaminants find themselves are simply to varied and have not been studied sufficiently to enable know values to be used. Thus, other means of developing the required data must be used (e.g., chemical modeling, expert judgement leading to simplifying, yet environmentally protective, assumptions).

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To determine the kinetic and thermodynamic constants required for the HWIR Assessment, each of the HWIR teams were queried to determine what their chemical-specific data needs were. Based on these discussions, the chemical-specific fate and data required for the HWIR Assessment are listed in Table I. It is anticipated that as the HWIR strategy develops further, that the data needs may require some revision.

Table I: Chemical-specific properties data set required fate and transport assessment.

Thermodynamic constants	**Kinetic constants**
Molecular Weight (g/mol)	Transformation Processes/Rates
Henry's law Constant (atm-m^3/mol)	Hydrolysis
Molecular Diffusivity in Air (cm^2/s)	Aerobic Biodegradation
Molecular Diffusivity in Water (cm^2/s)	Anaerobic Biodegradation
Solubility Limit in Water (mg/l)	
Octanol/Water Partition Coefficient	
Organic Carbon Partition Coefficient (ml/g)	
Speciation of Organics	
Ionization Constants (pKa values)	
Tautormerization equilibria	
Hydration equilibria	
Distribution Coefficient (Metals) (ml/g)	
Metal Complexation	

To generate all relevant chemical-specific data for the HWIR assessment, the use of measured, calculated and estimated data were necessary. Although measured data were preferred, the absence or scarcity of measured stat that are reliable necessitated the use of data that had been generated by computational methods. The SPARC (System Performs Automated Reasoning in Chemistry) model, which is a computational method based on fundamental chemical structure theory, was the primary tool for calculating the thermodynamic constants listed in Table 1. At the present time, SPARC does not have the capability of calculating molecular diffusivities in water. Because no other adequate computational or estimation method exists for this purpose, the generation of data for this parameter was limited to those

measured values that can be found in the literature. The SPARC model has already been used to calculate Kow values for approximately 200 HWIR chemicals. Because the Kow calculator in SPARC has been upgraded, it was necessary to recalculate these values.

Further development of the SPARC model has made it possible to predict the speciation of organic chemicals as a function of environmental conditions. Ignoring the possibility for speciation will potentially result in significant errors in the prediction of distribution and chemical reactivity of the HWIR chemicals that are subject to ionization, tautormerization and hydration. The HWIR chemicals that can speciate under environmental conditions were identified and the relative concentrations of the chemical species were estimated.

Kinetic Parameters

To the extent possible, first-order rate constants for hydrolysis and aerobic and anaerobic biodegradation were provided for each of the organic chemicals on the HWIR list. Because the process of assembling measured and estimated hydrolysis rate constants for the HWIR chemicals has been completed, recent efforts have and will continue to focus on developing the data set for chemical reduction and aerobic and anaerobic biodegradation. The chemical reduction and anaerobic biodegradation of organic chemicals in aquifers will be controlled to a large extent by the subsurface redox environment. In the past, the HWIR methodology has sidestepped the issue of properly representing groundwater redox conditions because existing data and methods for measuring redox status (platinum electrode measurements) are known to be critically flawed. Consequently, there has been a major weakness in determining the degradation rates of organic chemicals whose transformation pathways are dominated by redox reactions. This situation also applies to the transport of redox sensitive ligands. A long-term goal is to identify principal oxidizing and reducing chemical species in groundwater aquifer and sediments and their use for the prediction of the transformation of redox sensitive metals and organics. Although this research effort is considered long-term (3 to 5 years), it is fully anticipated that this ongoing research effort will provide immediate support for the team's effort in assembling a fate data base for the HWIR chemicals.

Charge to the Reviewers

The reviewers are requested to focus their efforts on critiquing our approach to constructing the HWIR fate data base. The SPARC model was thoroughly reviewed in FY97. Thus, further review of the model itself is not necessary, however, its application to the calculation of thermodynamic constants for the HWIR data base should be scrutinized. The computational methods outlined in the write up for the HWIR data base should be validated. Also, the reviewers are not being asked to check the accuracy of the individual numbers in the data base. We feel that this process is beyond the scope of this peer review process. EPA personnel are in the process of reviewing the data base for errors that might have occurred during the transcription of data.

Comments on the HWIR98 Research Plan
Chemical and Biological Fate Data Team

Dr. Dickerson:

Background: This section is well written and needs few scientific and no grammatical changes. I have taught chemodynamics for many years using a number of texts. In this class, we have taught students to calculate molecular diffusivities of chemicals in water and air. While it is true that calculation of molecular diffusivities in liquids is not as precise as for gases, the empirical correlation of Wilke and Chang may be used for nonelectrolytes in a variety of solvents:

$$D_{AB} = \frac{7.4(10^{-8})\,(\phi M_B)^{0.5}T}{\mu'\,\acute{\iota}_A^{\,0.6}}$$

There are correlations for strong electrolytes but these are much more complex to compute. However, the above equation is adaptable and should be considered.

Kinetic Parameters:
No errors found.

*Charge to Reviewers***:**
Wright up should be changed to write up.

Dr. DuPont: This document provides the background for the physical/chemical property data base effort required as part of the HWIR Risk Assessment process, defining the overall objectives and approaches that the Chemical and Biological Fate Data Team is taking in meeting their charge. An argument is made in the Background section that the complexity of the natural environment into which hazardous chemicals are released is so varied "...and have not been studied sufficiently to enable known values to be used." This statement seems to have justified the use of all estimated values in the HWIR Risk Assessment approach using the SPARC model, despite the fact that the SPARC model cannot calculate molecular diffusivities in water, and based on notes in the data base that indicate that it also cannot estimate the following: any parameters for inorganic compounds, no parameters for nitrosomine compounds, and no parameters for any phosphoric acid compounds or its derivatives.

Based on this background information it is not clear why the SPARC approach was chosen to be used for property estimation for the HWIR Risk Assessments. Many other methods exist, that have been documented, validated and peer reviewed, for the estimation of physical/chemical properties of chemicals relevant to HWIR Risk Assessments, and to the environmental media into which they would be released. There is also an extensive database of many of the chemical properties listed in Table 1 of this document, and I disagree with the statement on the first page of this document that suggests that known values cannot be used because of the variability of the natural environment. Much of this variability in natural systems is structural, i.e., the significant variability in permeability of aquifers and unsaturated zones, the significant variability in the distribution of contaminant following an uncontrolled release, the significant variability in the distribution of soil texture and native organic matter content within the native soils in which the chemicals are released, and scale dependent. The variability of chemical properties in many, many cases will have only a limited affect on the fate of a compound when released to the environment due to the overriding variability in the environmental properties themselves. I would argue that the effort in providing reliable risk assessments and fate and transport analyses for chemicals of concern in the HWIR should be focused not on chemical property issues, but on developing better descriptors for the physical/structural aspects of release sites that we only poorly describe and quantify at most sites.

As indicated above, many alternative, and peer-validated methods exist for estimating chemical properties listed in Table 1 of this document. One classic reference and compilation of a wide range of these methods of property estimation is the Handbook of Chemical Property Estimation Methods, Environmental Behavior of Organic Compounds by Lyman, Reehl, and Rosenblatt, published by McGraw-Hill, and is included in the reference list for the Physical/Chemical Properties of HWIR Chemicals document. The first edition was published in 1982, and the second edition was recently updated and republished in 1996. This handbook includes a variety of estimation methods for each of the properties in Table 1 except the speciation properties, and the metal distribution and complexation descriptors. Contrary to the statement made in this document regarding the estimation of molecular diffusivity values in water, even the 1982 edition of the handbook provides six methods for estimating diffusivity values in water with four of the six methods providing absolute average errors of estimated to measured values between 5.8 and 8.8 percent using an 87 compound database. Another classic reference is Chemodynamics by Thibodeaux, published by John Wiley & Sons. The first edition in 1979 has been updated in a second edition published in 1992. In this reference a wide variety of physical/chemical property estimation methods are described in the

context of the transport and fate of chemicals in environmental systems. The section in this text on diffusivity values provides four equations for the calculation or estimation of diffusion coefficients in air and water systems with accuracies of Ò 10%. This level of accuracy would definitely appear adequate for this variable due to the low values of this parameter for all compounds, and the relatively unimportant role diffusion in the aqueous phase plays in the overall transport of materials in the saturated zone. These are only two references that I frequently use for property data and for valid estimating approaches. There are many more documents available that summarize other validated studies and computerized property-property, property-structure, molecular surface area-property, etc., methods that would have seemed appropriate for inclusion in the HWIR Risk Assessment methodology. Many of these methods have been incorporated into other EPA-generated fate and transport or risk assessment approaches including the Hazardous Waste Treatment, Storage, and Disposal Facilities (TSDF) Air Emissions Models (CHEMDAT6), OAQPS, EPA-450/3-87-026, and the Superfund Exposure Assessment Manual, ORR, OSWER Directive 9285.5-1, EPA/540/1-88/001. While these documents are somewhat dated, the property estimation approaches they use are based on well documented, validated methods yielding property estimates that are within acceptable error for the purpose of exposure assessments from Superfund and TSDFs. Again, it is not clear why these existing approaches were not used in the HWIR process

There also exists a large database for many of the chemical properties listed in Table 1. One example of such a data pool include the OAQPS document listed above (EPA-450/3-87-026) which contains data for the following properties for most of the 743 compounds in its data base: molecular weight, density, vapor pressure @ 25⁻C and vapor pressure coefficients for calculation at other temperatures, aqueous solubility, Henry's Law constant, diffusion coefficient in water, diffusion coefficient in air, boiling point, cancer unit risk, allowable daily air intake, and ration of BOD to COD. A recent publication I was involved with, Innovative Site Remediation Technology, Design and Applications, Bioremediation, by Dupont, Bruell, Downey, Huling, Marley, Norris, and Pivetz, American Academy of Environmental Engineers, 1998, summarized physical/chemical properties of 71 of the most commonly found chemicals at Superfund sites based on data compiled by the U.S. EPA R.S. Kerr Laboratory in Ada, Oklahoma. The properties summarized in this document include the following: melting point, aqueous solubility, vapor pressure, Henry's Law constant, density, dynamic and kinematic viscosity, log Kow, log Koc, general biodegradability, and MCL. Based on the information available on many compounds of interest, I question

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the apparent deferral to predicted data over observed, measured data that is easily accessible in the open literature.

On a final note regarding this document, I completely agree with the statement made on the last page regarding the important role redox conditions play on the fate of contaminants in the subsurface. Based on the experience we have had evaluating natural attenuation of hydrocarbons and chlorinated solvents in groundwater systems at a variety of sites across the country, redox conditions are the primary control on contaminant degradation rates, and their subsequent movement away from the source of the release. This is particularly true for chlorinated alkanes, and a long-term effort to evaluate transformations of both organic and inorganic constituents under a variety of redox conditions would appear to be well directed.

The charge to reviewers is somewhat difficult to deal with as it requests that we not review SPARC, but only its application to the calculation of properties for input to the HWIR data base. I attempted to find some validation of the model in the referred literature and found very little for other than ionization constant estimation. One paper by Bouchard (Sorption kinetics of PAHs in methanol-water systems, Contaminant Hydrology 34(1-2):107-120) addresses peripherally the use of SPARC for the prediction of desportion rate constants via a SPARC prediction of Kow. SPARC estimated values for the log of this desorption rate constant were within 16 to 23%, bringing into question the accuracy of this SPARC estimation method. Was the model validated and reviewed prior to this point for all of the properties included in the data base? I would expect that other available methods would provide desportion rate estimates as accurate as SPARC did for the PAH compounds in Bouchard's study, so where is the justification for the use of SPARC generated property data for all compounds in this HWIR data base?

Comments on Physical/Chemical Properties of HWIR Chemicals

Dr. Dickerson:

SPARC Models

It is my opinion that a brief description (approximately one paragraph) would aid of the document understanding. The first reaction to SPARC by my colleagues was a workstation and programs by SUN. At the very least, the acronym should be defined.

The authors should ensure that the same symbols are used for the equation and text description. For example, in the first equation, different symbols are used for sigma in the equation and text accompanying the equation.

SPARC Physical Models

In the first equation, it should read delta G monomer instead of monmer. In my opinion, there is insufficient detail in this section. No mention is made of the terms for delta G interaction in the gas phase. However, the approach appears correct based on the information supplied.

Dr. DuPont: The approach that was used in the Physical/Chemical Properties of HWIR Chemicals data base described in this document is not clear at all, and the benefits of SPARC over other property estimation approaches is not at all elucidated in this discussion. It is totally unclear how SPARC generated estimates of compound reactivity are related to measured chemical properties that SPARC is estimating so that the method can be validated. All that is indicated in the discussion on Page 3 is that SPARC reactivity parameter estimates were fitted to various governing expressions described on Pages 4 through 11, to generate coefficients in the computerized database. For the many compounds and properties that have measured and reported values in the literature, why weren't these values put into the database with corresponding temperature corrections applied for site-specific conditions? How can the use of model-predicted values be justified when measured values are available?

The advantages of making temperature dependence "...intrinsic to each core interaction model as opposed to algorithmically described at the property level." as described on Page 4 of this document are not stated at all. This incorporation of temperature dependence into the property descriptor seems to only eliminate the use of measured values, and is questionable in terms of the benefits it provides to the estimation process in terms of the costs that result from not using real data. It is not clear why measured properties are not fitted to the proposed algorithms instead of the SPARC estimated values as was apparently done with water viscosity.

The approach used for molar volume, gas diffusion coefficient, and vapor density, while consistent with the other fitting equations do not seem appropriate based on the Ideal Gas Law. Molar volume should be directly proportional to absolute temperature, with the coefficient being determined from the product of the

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number of moles times the gas constant, R, divided by pressure. The diffusivity value in gas should have a 3/2 coefficient based on the Chapman Enskoy formula (Thibodeaux, 1979), and vapor density should be inversely proportional to absolute temperature times a constant defined by the ideal gas constant divided by pressure. None of the expressions presented on Page 9 are in the form they should be, and the reasons for this, other than to keep all the fitting equations the same, needs to be stated.

It remains unclear whether aqueous diffusivity values are included in the data base or not. The HWIR98 Research Plan document indicates that the SPARC model can't estimate diffusivity in water, while an equation for estimation of this property is presented on Pages 11 and 12 of the Physical/Chemical Properties Document. Which is it?

The approach for the incorporation of transformation process data into the data base appears adequate to a point. For the hydrolysis rate constant effort, the approach to identify and generate rate data via literature and laboratory measurement appears good, but the generation of all property values for hydrolysis products using SPARC rather than measured values is once again a problem. Generating properties using SPARC somehow without validation does not seem reasonable at all.

The aerobic degradation database consisting of only 23 compounds is very inadequate. I am not familiar with the SRC report referenced on Page 14, but I know there are aerobic degradation rate data for more than 23 compounds available in the literature for soil, water, and sediments that fit the criteria stated on Page 15. Should this number be 230? or 2,300? There must be more than 23 values based on the stated number of compounds from the BIOLOG (7,820 compounds) and DATALOG (15,965 compounds) data files in SRC's environmental fate data base. When this number is whittled down to 10 chemicals based on mineralization rate constants it seems impossible that only this small number of compounds have reported mineralization rates when the search began with a field of nearly 24,000 compounds. This needs to be looked at carefully. We have generated dozens of aerobic degradation rate constants in aerobic soil systems for the R.S. Kerr Laboratory that have been incorporated into several EPA documents, one of which includes the following: Treatment potential for 56 EPA listed hazardous chemicals in soil. 1988. U.S. EPA Office of Research and Development, RSKERL, Ada, OK. EPA/600/6-88/001. R. C. Sims, W. J. Doucette, J. E. McLean, W. J. Grenney, and R, R, Dupont. The Hazardous Waste Treatment, Storage, and Disposal Facilities (TSDF) Air Emissions Models (CHEMDAT6), OAQPS, EPA-450/3-87-026

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document has first-order rate constants reported for six compounds in two soil environments on Page 5-34, and the model, CHEMDAT6, has aerobic degradation rates for dozens of compounds in aqueous systems.

The values that do appear in this Physical/Chemical Properties of HWIR Chemicals data base generally have ranges such as 0.025 to 7.3/d for acetone, making them virtually useless for fate and transport modeling as they vary over a reported range of more than two orders of magnitude. To make these degradation rates useful, some designation of the environment in which the rate is reported should be defined, i.e., aerobic rates in surface soils should be differentiated from aerobic rates in surface water, should be differentiated from aerobic rates in ground water, as these rates would be expected to vary greatly from one medium to another due to mass transfer limitations, microbial population levels, environmental stresses, etc.

There is no discussion at all in this document regarding anaerobic degradation rates. A great deal of literature has been published in the last several years regarding contaminant (primarily aromatic hydrocarbons and chlorinated alkanes) degradation rates in aquifer systems under a variety of alternative electron acceptor conditions in response to the investigation of the applicability of natural attenuation at many sites. These values should be collected and incorporated into this data base to take advantage of the work that is building in this area.

The Computerized Database

The electronic file that I was sent was readable in Excel98, but column headings were only provided for the compound name, CAS number, SMILES string, molecular weight, and chemical boiling point. Several of the reaction rate value columns could be identified on the far right of the sheet, but these entries were sparse. All of the other columns were either cryptic (YC?) or not labeled at all. No calculational methods were included in the cells either, so no differentiation could be made between measured values, and those estimated using SPARC. It remains unclear whether these data were used to calibrate and validate SPARC estimated values, or whether these values are just a tabulation of non-validated SPARC estimates with no validation whatsoever. If the later is the case, the use of this data base is highly questionable, particularly when it is to be applied in a risk assessment context for the HWIR.

Summary

I had major questions and concerns regarding these documents as evident from my comments above. Questions arise regarding the validity of the SPARC model for the wide range of properties listed in Table 1 of the HWIR98 Research Plan document. Major questions remain regarding the approach that was used to generate coefficients for the HWIR database. I do not understand why known, measured, reported property data were not used in place of estimated values from the SPARC model. I do not understand why property values presented in other EPA documents, generated by other EPA laboratories, and reported in the open literature were not incorporated into this database. I do not understand the advantage of using computer generated data as input into another computerized transport model when measured data exist. I would like to have seen some discussion of the error associated with model predictions and the propagation of error when using these parameters in typical fate and transport models. I would also have liked to see some discussion regarding the relative importance of chemical property variability versus site/soil variability when carrying out risk assessments at typical sites.

Much of the material I read was unclear and confusing, and did not do a good job of justifying the use of what appears to be an unvalidated, in-house, property estimation model that does not appear to be any more accurate or easy to use than the myriad of estimation approaches that are currently available in the literature. It would make more technical sense to utilize available measured data first, then estimation methods from the literature for those properties for which they have been validated, then use SPARC for the speciation properties for which it has been validated in the literature. In this way, the validity and confidence of the data and properties estimated from the data can be maximized for the important end purpose of conducting risk assessments for HWIR chemicals.

Dr. Linkov: *GENERAL COMMENTS*

The HWIR fate database will be used for exposure and risk assessment across a wide range of environmental settings and for a wide range of chemicals of concern. Since the HWIR fate database will be important for making policy decisions, scientists and decision-makers should be provided with enough information to evaluate the interpretation of the data collected from the literature and/or experts. This is particularly the case for the data generated by SPARC (see below). Uncertainty associated with the experimental or measurement procedures and/or calculations should be reported in the database. Variability due to environmental conditions should be reported for measured data in the database.

The interim report proposes extensive use of the SPARC model since measured data for physical/chemical properties are not available for many of the HWIR chemicals. Use of any structure-activity software for prediction is valid insofar all potential shortcomings of the approach are considered. If the database is used for risk assessment without critical examination of all uncertainties associated with parameters generated by the SPARC model, there is the possibility that the data will be presented as more precise or empirical than is actually the case. Dr. M. Nendza concludes her 1998 book on "Structure-Activity Relationships in Environmental Sciences" with the following statement: "QSARs can be good tools for generating data, but their interpretation remains the responsibility of the scientist." The input data for SPARC should be readily verifiable for every calculated parameter to provide unbiased data interpretation.

Even though the interim report presents a solid and scientifically sound method to constructing the HWIR fate database, the applicability of the database for risk assessment may be limited if the user is unable to assess the uncertainty and limitations of the input data and model algorithms.

SPECIFIC COMMENTS

SPARC Models, SPARC Physical Models, OSW Algorithms

The SPARC model has already undergone a thorough review. However, the description of the interaction between the SPARC model and the OSW algorithms is not clearly presented in the interim report. It is not readily apparent exactly what comprises the output of the SPARC model and how specifically that output is used in the OSW algorithms. This early introductory section should be clarified.

General Model

The OSW model applies the theory of acid-base equilibrium to calculate the pH dependence of particular thermodynamic properties. This theory is generally applied in analytical chemistry for such models. Combined with the hydrolysis model, it represents the proper state of the chemicals at different pH states.

The OSW model assumes linear dependence of corresponding equilibrium constants on inverse temperature for thermodynamic equilibrium process parameters such as pKa, Henry Law constant, K_{ow}, solubility, etc. (equation 1, p.4). Often in the literature, this is assumed or verified to be true (for example, change in partial pressure with temperature for some organic compounds [Gucker, 1966]). In some cases, however, experiments have revealed a deviation from linearity, which is explained by the significant temperature

dependence of ΔH^{o} (for example, solubility in water of organic enanthiomers [Pudipeddi et al, 1995] and chemical reactions in water and organic solvent [Liu et al, 1997])**.**

Even though the proposed algorithms are likely valid for the specified temperature range (0-60°C) for many of the HWIR chemicals, for some of them or some of the reaction products this assumption may be not valid. The questions of non-linearity of the temperature dependence of equilibrium constants are further addressed in Flynn (1997).

Ionization, Henry's Law Constant
I would like to leave comments on these issues to scientists with more experience in these issues.

Solubility and K_{ow}
The neglecting of transfer of ionic species into organic phase (octanol) is reasonable for the calculations for the HWIR fate database (Nendza, 1998 p.35).

Molar Volume, Gas Diffusion and Density
I would like to leave comments on these issues to scientists with more experience in these issues.

Sorption.
Experimental sorption data varies considerably because it is governed by both soil and contaminant properties. Extrapolation of sorption coefficients obtained for one soil type to another is inappropriate since the sorption capacity of soils may range over several orders of magnitude for the same compound (Nendza, 1998). Therefore, it especially important to be able to trace the original data used in the derivation of the specific sorption parameters.

Moreover, many QSAR relationships used for the sorption estimation are based on a specific class of compounds (pesticides, non-polar aromatic compounds, esters etc.) and are not generally applicable to the other classes (Nendza, 98 p.112). The HWIR database lists compounds from various classes. Therefore, it is important that either the model employed should be demonstrate validity over a wide range of chemicals or the QSAR algorithms should be specific to the chemical under consideration.

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The proposed algorithm uses the following relationship between K_{oc} and K_{ow}:

$$\log K_{oc} = a(\log K_{ow}) - b$$, where a=1 and b=-0.32

Significant ranges of variation (0.8-1 for a and –0.35 -- +0.29 for b) were reported for non-polar aromatics, and these coefficients can be very different for more polar chemicals (Nendza, 98 p.111). Majority of the chemicals (more than 200) in the HWIR list that I received are polar (examples are acetaldehyde, methanol, ethoxyethanol, nitrobenzene etc.). Therefore, it seems likely that different algorithms should be proposed for such chemicals.

Transformation Processes and Technical Approach

The technical approach implemented for construction of the HWIR fate database involves extensive literature review, expert judgment elicitation and modeling and is in general scientifically and technically sound. The data-quality requirements are especially crucial for deriving sound QSAR models and therefore for the use of all information derived with the QSAR models. Since the experimental data is collected from different media and show significant variation, the data used for specific calculations should be easily traced through the database. The specific suggestions are as follows:

Data presentation

Data should be converted and reported in the same units and clearly labeled. The version of the database that was received for this review has many unlabeled fields and units are often not given. Experimental data should be clearly distinguished from calculated values and expert judgments. For experimental data, media and experimental design should be reported. Specifically, the time course of the experiment should be reported because short-term experiments often report transient data rather than equilibrium characteristics.

Uncertainty

Estimates of the data variability and uncertainty (such as range and/or standard deviation) should be presented along with the 'best' estimate. Variability should be distinguished from uncertainty where possible.

Data Visualization

All QSAR models used in the database should be accessible for visual graphical examination with all data points used, including outliers.

Environmental Factors

Environmental conditions and release routes and rates should be reported for field experiments. Both the physical properties of the chemical under consideration and the environmental conditions under which the chemical is evaluated both play major roles in the ultimate fate of the chemical in the environment.

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