UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

JAN 12 2005

OFFICE OF
ENVIRONMENTAL INFORMATION

Mr. William L. Kovacs
U.S. Chamber of Commerce
1615 H Street, N.W.
Washington, D.C. 20062

Dear Mr. Kovacs:

This letter responds to your May 26, 2004, Request for Correction (RFC) of physical and chemical property information contained in the Environmental Protection Agency (EPA) databases under the *Guidelines for Ensuring and Maximizing the Quality, Objectivity, Utility, and Integrity of Information Disseminated by the Environmental Protection Agency* (Information Quality Guidelines or IQGs). In your RFC you state that 16 databases listed in Section I of the RFC (hereafter referred to as EPA databases) are not consistent with the EPA IQGs because they contain ". . . inconsistent and contradictory numerical data entries for physical-chemical constants characteristic of various chemicals that are used in commerce or that occur in the environment." The RFC lists a number of chemicals found in one or more EPA databases and asks that EPA "assure that the databases consistently and uniformly indicate the same, correct numerical value for any listed physical or chemical property parameter associated with the identified chemicals." EPA has reviewed your RFC and determined that the existing EPA databases and models referred to in your RFC individually are in conformance with the EPA Information Quality Guidelines. However, two actions have been taken as a result of your RFC. (1) Two sentences were added to the PBT Profiler web page to clarify the appropriate use of data from the Profiler; and (2) The Soil and Transport Fate (STF) database was temporarily removed from the web site for review to make sure that the information complies with the Information Quality Guidelines. The database will not be re-posted until the review is complete and any necessary modifications have been made. The other items listed in your RFC have either been superseded by other databases and therefore, no longer exist on the EPA web site or are not EPA databases. The detailed results of the EPA review of the RFC list of items are in an attachment to this letter.

There are valid reasons why databases may contain differing values for physical or chemical parameters. A specific property value for the same chemical may differ due to site-specific circumstances, as your letter acknowledges, and will also depend on the source of the information and the methodologies used. This is especially true when deciding the most

appropriate value to use in a particular model. With respect to EPA databases and models, EPA fosters information objectivity by clearly explaining the purpose and intended use of the database or model in its public presentation and providing appropriate documentation on the sources of the information provided.

Regarding the use of data in EPA databases, EPA cautions that, contrary to the assertions in the RFC, data from EPA databases may not be suitable for use in all situations. The EPA databases cited in the RFC do not predetermine the outcome of any rulemaking or other Agency action. When EPA uses such information to support a rulemaking, the scientific basis for, and the application of, that information are subject to public comment as well as to EPA's data Quality System and Peer Review Policy. Consistent with the IQGs, the quality of information in any individual rulemaking or Agency action should be scaled and appropriate to that use.

If you are dissatisfied with EPA's response, you may submit a Request for Reconsideration (RFR). EPA recommends that this request be submitted within 90 days of the date on this letter. To do so, submit a written request to the Agency's Information Quality Guidelines Processing Staff via email at quality@epa.gov, by mail at US EPA, 1200 Pennsylvania Avenue, N.W., Mail Code 2811R, Washington, D.C. 20460. The request for reconsideration should reference the request number assigned to the original request for correction (RFC #04019). Additional information that should be included in the request is listed on the IQG web site at http://www.epa.gov/quality/informationguidelines.

If you have any questions concerning this response please contact Reggie Cheatham at (202) 564-6830.

Sincerely,

Kimberly T. Nelson
Assistant Administrator and
Chief Information Officer

cc: Henry Longest, Acting Assistant Administrator
Office of Research and Development
Thomas Dunne, Acting Assistant Administrator
Office of Solid Waste and Emergency Response
Susan Hazen, Acting Assistant Administrator
Office of Prevention, Pesticides, & Toxic Substances
Jeffrey Holmstead, Assistant Administrator
Office of Air and Radiation

ATTACHMENT

Status of Data Bases Identified in the U.S. Chamber of Commerce Request for Correction (RFC #04019)

Chemdat8 Superseded by Water9 as described on the Water9 web page at http://www.epa.gov/ttn/chief/software/water

CHEM9 Superseded by Water9 as described on the Water9 web page at http://www.epa.gov/ttn/chief/software/water

SIMS Surface Impoundment Modeling System. Superseded by Water9.

Water9 WATER9, a wastewater treatment model, is a Windows-based computer program and consists of analytical expressions for estimating air emissions of individual waste constituents in wastewater collection, storage, treatment, and disposal facilities; a database listing many of the organic compounds; and procedures for obtaining reports of constituent fates, including air emissions and treatment effectiveness.

Water9 Version 2 was released July 1, 2004. Significant internal and external review was done on Water9 Version 2. Duplicate compound entries with multiple names were eliminated. Compounds are now listed by the CAS number and their primary name. The WATER9 model contains a detailed agreement for user acceptance that must be acknowledged before the user may access the WATER9 database and the WATER9 compound property estimating software. This agreement indicates that the WATER9 information is not provided with any government assurance of accuracy, completeness, or usefulness, and that the user agrees to provide feedback to EPA for any problem that was noted. EPA worked extensively with the American Chemistry Council to obtain the best compound properties available for inclusion in the WATER9 database. The compound properties listed in the WATER9 data base are obtained from a variety of sources, including proprietary data bases such as the Design Institute of Physical Properties (DIPPR911) of The American Institute of Chemical Engineers, AIChE. When the Henry's law constant value for a specific compound in the WATER9 data base is viewed, the reference (such as DIPPR911) is also presented, as a condition of the use of the DIPPR data in the WATER9 data base.
There is also an understanding in the use of the specific compounds listed for Henry's Law constant values in the WATER9 program, that this compound property will not be a single value, but will be adjusted for site specific conditions, such as temperature, concentration, pH, oil content, organic carbon content, and other factors. Such deviations from a single compound property value and the

basis of the deviations are provided to the user as part of the WATER9 reporting system.

As a result of the uncertainty of compound property values and the lack of measured values for the many compounds of interest, WATER9 provides several different methods to estimate compound properties. The results of these different methods of compound property estimation can be viewed by the WATER9 user in the compound property window. When the user accesses the automatic compound property estimating procedures in their project, a warning must be acknowledged by the user that states: "Remember that the estimation procedures can result in inaccurate properties for some compounds. Accurate measured values for your system should be used whenever possible."

Some compound properties are not system specific such as pure component vapor pressure and molecular weight. Values in the WATER9 data base are corrected when more accurate information is available.
http://www.epa.gov/ttn/chief/software/water

PBT Profiler Persistent, Bioaccumulative, and Toxic Profiles Estimated for Organic Chemicals On-Line (http://www.epa.gov/oppt/pbtprofiler/). The PBT Profiler is a screening level model designed to evaluate chemicals lacking experimental data to help identify Pollution Prevention (P2) opportunities. The following two sentences were added to the "Purpose of the PBT Profiler" web page (http://www.pbtprofiler.net/notice.asp) to clarify the appropriate use of data from the Profiler: *"EPA does not use the PBT Profiler to assess and identify new chemicals submitted as PreManufacture Notices (PMNs) under the Toxic Substances Control Act, as being in the New Chemicals Category for Persistent, Bioaccumulative, and Toxic Chemicals. Professional judgment of EPA OPPT subject matter experts is used to assign PBT concern levels to PMNs"*. The PBT Profiler does contain the same computer models used by EPA to screen PMNs for "P" and "B". However, for PMNs "T" is determined by EPA OPPT human health experts using nearest analog analysis and is based on chronic oral systemic toxicity to humans, mammals, and birds. Measured data always takes precedence over screening model estimations. The PBT Profiler provides estimates of PBT characteristics, and is useful for establishing priorities for chemical evaluation when chemical-specific data are lacking. When a user accesses the PBT Profiler on the Internet, descriptions of the purpose and limitations of the model must be acknowledged before the user can access the model itself.

Several models that form the PBT Profiler (AOPWIN™, HENRYWIN™, and KOWWIN™) have measured data sets incorporated into them, and when a chemical is run through the PBT Profiler, these models will first search for measured data, and if no data are available for that chemical, the value will be estimated. Additional information on the methodologies used by the PBT Profiler

and the experimental data contained within the model is available at http://www.pbtprofiler.net/methodology.asp. Information on the specific model components of the PBT Profiler is contained in the "Help" files of each model, which can be accessed by down loading and installing the integrated set of models, EPISuite™, at no cost from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm. The limitations of the PBT Profiler are highlighted and explained for the user within the model itself, which is located at http://www.pbtprofiler.net/.

KOWWIN™ The KOWWIN™ program, part of EPI Suite™, estimates the log octanol/water partition coefficient of organic chemicals using an atom/fragment contribution method developed at Syracuse Research Corporation. EPI Suite™ provides users with estimations of physical/chemical properties and environmental fate properties. Before using the EPI Suite™ models to estimate these properties, one should first determine whether any suitable data are available in the literature (e.g., Merck Index, Beilstein); this is facilitated by a database of 25,000 chemicals included in the EPI SuiteTM software. KOWWIN™ will first search for measured data, and if no data are available for that chemical, the value will be estimated. The User's Guide includes references to methodology used and an appendix on the estimation accuracy of KOWWIN™ (http://www.epa.gov/oppt/exposure/docs/episuitedl.htm). The OPPT Exposure Assessment Tools and Models web site has relevant information regarding intended use of estimated values. Representative measured values are preferred, and should be used when available. Measured values or estimates of water solubility and vapor pressure are important in evaluating whether a chemical will dissolve in water or exist as a vapor at ambient temperature, and are used to estimate worker and consumer exposures. Measured data or estimates of biodegradation, sorption, and volatilization potential are used to predict removal in wastewater treatment. Information on decay rates in the atmosphere, surface water, soil, and ground water are important in evaluating how long it takes a chemical to break down in the environment, and are used to estimate exposures to the general population and the environment. http://www.epa.gov/oppt/exposure/docs/exposurep.htm.

STF Soil and Transport Fate Database. STF is a computer-based tool for selecting data on chemicals in the environment and for simulating their fate and transport in site-specific conditions. This database has been removed from the EPA web site pending review of the data contained in the database. The software consists of three components: the Soil Transport and Fate Database (STF 2.0), two screening level models (RITZ and VIP), and a user interface connecting the database with the models. The STF 2.0 database provides information on the behavior of chemicals in soil environments for use as input data on, for example, degradation rates and partition coefficients. The RITZ (Regulatory and Investigative Treatment Zone) model simulates unsaturated zone flow and transport of oily wastes during

land treatment. The VIP (Vadose zone Interactive Processes) model is a one-dimensional finite-difference solute fate and transport model for simulating the behavior of organic compounds in the vadose zone as a part of a land treatment system. EPA is reviewing the database incorporated in the STF software package to determine the accuracy of the data contained therein. Upon completion of the review, a decision will be made as to whether or not the database will be once again made available. In the meantime, users of the database are advised that, while the information in the database is believed to be reliable, neither EPA nor any of its contractors make any further claim to the accuracy of the data and are not responsible for any use made of the data nor any consequences arising from such use. http://www.epa.gov/ada/csmos/models/stf.html

SCDM Superfund Chemical Data Matrix. SCDM is a database containing factor values and benchmark values used for applying the Hazard Ranking System (HRS) rule to evaluate potential National Priorities List (NPL) sites. Input data are taken from EPA developed literature sources and databases and/or peer reviewed literature sources and databases. The accompanying SCDM Methodology report describes how data are selected or calculated for inclusion in SCDM and how SCDM data, HRS factor values, and benchmarks are presented in formatted printouts. SCDM was updated in 2004.
http://www.epa.gov/superfund/sites/npl/hrsres/tools/scdm.htm

SCDM Win SCDM Win was a Windows-based user interface for the 1996 version of SCDM. SCDM Win is not usable with the current version of SCDM (2004) and is no longer supported.

SPHEM Superfund Public Health Evaluation Manual, EPA/540/1-86/060. Superseded by the Risk Assessment Guidance for Superfund, EPA/540/1-89/002, December 1989. http://www.epa.gov/superfund/programs/risk/tooltrad.htm

HHRP Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities EPA/530/D-98/001A. Draft guidance document. The physical/chemical parameters are taken when available from the Superfund Chemical Data Matrix (SCDM). Documentation for all physical chemical parameters are provided in the guidance. The parameters in the guidance are a snapshot of what was current in 1998 when the draft document was developed. When the guidance is finalized these parameters will only be current as of the date of that publication. The Peer Review Draft is available at:
http://www.epa.gov/epaoswer/hazwaste/combust/risk.htm

TREAT DB The Treatability Data Base (version 5.0, 1994) provides a review of the removal/destruction of chemicals in various types of media, including water, soil, debris, sludge and sediment. The treatability data summarizes the types of treatment used to treat specific compound, the type of waste/wastewater treated, the size of the study/plant, and the treatment levels achieved. The sources for the physical/chemical property information in the Treatability DB are taken from existing sources and are cited and fully documented in the database. The user is given a standard library citation and then a brief abstract of the source material. The database contains a disclaimer that data in the database are a tabulation from many sources and are presented for review by the user for informational purposes only. The data presented does not represent a total listing of the technologies capable of treating the target chemical compound and should not be viewed as solely reliable for treatability system design and should be thoroughly reviewed to support regulatory guidelines. Therefore, the conclusions and opinions drawn are solely those of the user and are not necessarily the view of the Agency. The database is available on disk from http://www.epa.gov/ORD/NRMRL/treat.htm.

PhysProp Syracuse Research Corporation. PhysProp is not an EPA database and is therefore not subject to correction by EPA. This database is among the sources used in SCDM, the PBT Profiler and EPI Suite™ (includingKOWWIN™). Quality control on the PhysProp database is performed by Syracuse Research Corporation using a multi-step peer review process. http://www.syrres.com/esc/physprop.htm

Chemfate Syracuse Research Corporation. Chemfate is not an EPA database and is therefore not subject to correction by EPA. This database is among the sources used in SCDM. Recommended values in Chemfate come from PhysProp. Quality control on the Chemfate database is performed by Syracuse Research Corporation using a multi-step review process. http://www.syrres.com/esc/efdb.htm

ATDSR It is likely this refers to the last line of Table 1 in Attachment 1 of the RFC (Peer Review Draft of article "*Uncertainty in K_{ow}..*" by Linkov, Ames, and Crouch), where the reference cited is *Toxicological Profile for Polychlorinated Biphenyls (PCBs),* published November 2000 by the Agency for Toxic Substances and Disease Registry (ATSDR), which is part of the US Department of Health and Human Services, US Public Health Service. We did verify that the value noted comes from Table 4-3, page 454, of the document and the references cited are not EPA documents.

RCRA We have been unable to identify this database from the information provided.