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

JUN 22 2007

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

**RE: Request for Reconsideration (RFR) of the U.S. Chamber of Commerce's Request for Correction (RFC) of Databases and Models (RFR #04019A)**

Dear Mr. Kovacs:

This letter is in response to the U.S. Chamber of Commerce's (Chamber) Request for Reconsideration (RFR) received by the United States Environmental Protection Agency (EPA) on April 11, 2005. The Chamber requested that EPA reconsider its response to the Chamber's Request for Correction (RFC) of information about the properties of various chemicals that are available in certain EPA and privately-owned databases and models. The Chamber believes that the information disseminated in the databases and models is not consistent with the Information Quality Act (IQA), the Office of Management and Budget *Guidelines for Ensuring and Maximizing the Quality, Objectivity, Utility, and Integrity of Information Disseminated by Federal Agencies*[1] (OMB IQG), and the EPA *Guidelines for Ensuring and Maximizing the Quality, Objectivity, Utility, and Integrity of Information Disseminated by the Environmental Protection Agency*[2] (EPA IQG). In response to your RFR, the executive panel concludes that there are valid reasons why databases may contain differing values for physical or chemical parameters. Nonetheless, in response to your request, the Agency has conducted a thorough review and has made a number of improvements to EPA Web sites to enhance the objectivity, utility and transparency of information in some of its databases and models.

As described in the EPA IQG, EPA convened an executive panel to consider the Chamber's RFR. The executive panel for this RFR was comprised of myself, the Regional Administrator for EPA Region III, EPA's Acting Science Advisor,[3] and EPA's Economics

[1] 67 Fed. Reg. 8452 (February 22, 2002). http://www.whitehouse.gov/omb/fedreg/reproducible2.pdf
[2] 67 Fed.Reg. 63657 (October 15, 2002).
http://www.epa.gov/quailty/informationguidelines/documents/EPA_InfoQualityGuidelines.pdf
[3] The panel was convened in December 2005. The Acting Science Advisor served on the panel because EPA's current Science Advisor was not appointed until January 25, 2006. The current Science Advisor did not participate in the panel. The Acting Science Advisor is no longer with the Agency.

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Advisor. During this meeting, the executive panel was informed of activities initiated to address the Chamber's concerns. In its RFR, the Chamber requested correction of certain information it had identified as faulty and raised the following concerns:

1. The Chamber alleged that EPA's use of Web site notifications to alert potential data users of the limitations of certain data disseminated on EPA Web sites and to suggest appropriate uses for the data is contrary to the IQA, as well as the EPA IQG.

2. The Chamber asserted that it was inconsistent with the EPA IQG for EPA to recommend the use of certain data on privately-owned Web sites without assuming responsibility for the quality or correct usage of that data.

3. The Chamber recommended that the data quality concerns it raised be addressed through an inter-agency review process, to improve the accuracy and consistency of data disseminated by government agencies.

**Panel Conclusions:**

In response to the Chamber's request for EPA to reconsider its response to the RFC, the executive panel concludes:

1. There are valid reasons why databases may contain differing values for physical or chemical parameters.

2. The Agency should continue to enhance its efforts to implement and improve policies and procedures for addressing life cycle management of data and databases. (The System Life Cycle Management policy[4] issued by the Agency's Chief Information Officer should address these issues. The subsequent development of procedures, standards, and guidance to support this policy will describe EPA's practices for addressing superseded databases. These procedures and standards should also identify the activities associated with periodic risk assessments and testing to ensure that errors are not propagated from one database to the next.)

3. There would be a potential benefit to the Agency from participation in an interagency workgroup that evaluates the quality of data being used across the federal government. The Agency should look for opportunities to work with other federal agencies to address data quality issues.

[4] EPA Information Policy, EPA Classification No. 2100.5, CIO Transmittal No. 06-009, April 7, 2006. http://www.epa.gov/irmpoli8/ciopolicy/2100.5.pdf

**Actions Taken by EPA in Response to the Chamber's RFR**

Since the receipt of your RFR, EPA has taken a number of actions to address the concerns raised by the Chamber about the "objectivity," "utility," and "integrity" of the information disseminated in EPA databases and models and in two privately-owned databases. EPA has updated the EPA databases and models to describe data limitations, suggest appropriate uses for the data, and, where appropriate, offer a range of values, instead of one value. EPA has also clarified or updated certain information in these databases and models. Two of the databases identified by the Chamber, PhysProp and CHEMFATE, are owned by the Syracuse Research Corporation (SRC). SRC made improvements to the PhysProp and CHEMFATE databases at EPA's request. These improvements included reporting a range of values in the CHEMFATE database. Appendix A describes other improvements that were made to the databases and models being disseminated by EPA and SRC. Appendix B provides a description of the attributes that contribute to the objectivity, utility, integrity, and transparency of this information.

In response to the Chamber's request that EPA participate in an inter-governmental multi-Agency workgroup to address the concerns the Chamber raised about data quality, EPA contacted the co-chair of the National Science and Technology Council (NSTC) Digital Data interagency working group. Upon further discussions with the NSTC co-chair, EPA learned that this workgroup will not specifically address the concerns raised in the Chamber's RFR. EPA recognizes the merits of further efforts in this area and the Agency plans to look for opportunities to work with other Federal agencies to address data quality.

**EPA Processes that Ensure Information Quality**

EPA has established processes to ensure and maximize the quality of information it disseminates. Examples of these processes include EPA's Quality Management System,[5] and Peer Review Policy and Handbook.[6] These processes provide for independent review and public participation in Agency decisions. To ensure that information is not misused or misunderstood, EPA also uses cautionary statements and disclaimers to notify users of the quality and potential limitations of disseminated information. In addition to these processes, in May 2000, EPA launched the Integrated Error Correction Process (IECP).[7] The IECP affords the public an opportunity to propose corrections to data that are posted by EPA's information owners, including discrete numerical values in EPA's databases. Since its inception, 90% of the notifications received through IECP have been resolved by EPA.

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[5] EPA's Quality System for Environmental Data and Technology. http://www.epa.gov/quality/index.html

[6] EPA Science Policy Council, Peer Review Handbook - 3rd Edition, EPA Document Number 100B06002. http://www.epa.gov/peerreview/pdfs/Peer%20Review%20HandbookMay06.pdf

[7] EPA Integrated Error Correction Process Web page: http://oaspub.epa.gov/enviro/ets_grab_error.smart_form?P_CALLER_URL=http://www.epa.gov/epahome/comments.htm Or locate the error correction process by going to the EPA Home Page at "www.epa.gov," then to "Contact Us" and then to the bottom half of that page to "Report Data Errors", or the URL: http://oaspub.epa.gov/enviro/ets_grab_error.smart_form

**Summary**

EPA believes the information in its disseminated databases and models is appropriate for its intended use, and we continue to promote transparency to prevent the misuse of information. The actions taken in response to the Chamber's RFR support the Agency's continuing efforts to ensure the quality, transparency, and reproducibility of the information in the databases referenced in this RFR. EPA will continue to implement policies and procedures that enhance the quality of information in our databases and models.

Sincerely,

Donald S. Welsh
Regional Administrator, Region III

Enclosures

cc: Molly O'Neill, Assistant Administrator, Office of Environmental Information
Brian F. Mannix, Associate Administrator, Office of Policy, Economics and Innovation
George Gray, Assistant Administrator, Office of Research and Development
Linda Travers, Deputy Assistant Administrator, Office of Environmental Information

**Appendix A: Actions Taken in the EPA databases identified in the Chamber's RFR**

**Chamber Request:** Improve the accuracy and consistency of data in the KOWWIN™, PBT Profiler, SCDM, WATER9, PhysProp, and CHEMFATE databases and improve the transparency of variability and uncertainty in the data included in databases.

**EPA Response:** EPA evaluated the data for polychlorinated biphenyls (PCBs) in the databases cited by the Chamber. EPA extensively investigated each perceived inconsistency between databases, and noted that these slight variations in assessment values between tools are not errors. In the absence of available measured data on chemicals of interest, predictive methods and structure-searchable databases can be employed to help the user characterize the physical-chemical properties and potential environmental fate of chemicals using the assessment tools noted above. To make a chemical estimate using tools such as EPI Suite™ and the PBT Profiler, a discrete chemical structure (referenced either by CAS number, name, or direct structural input) is required from the user in order to perform model calculations. Several of the commercial products on the market today, although represented by a single CAS number, are complex mixtures comprised of multiple chemicals with varying molecular structures. In these cases, these discrete CAS numbers can actually represent mixtures of chemicals, not single molecules, such as with mixtures of polychlorinated biphenyls. Use of the term PCB is a generic reference to structures that have common backbones, but varying numbers of chlorine atoms attached to the outside. Within a PCB mixture, some molecules can have as few as one chlorine atom, or many atoms attached. When the user inputs data to these tools using only CAS numbers as the initial chemical identifier, the model is programmed to review the CAS input, determine that the CAS number represents a mixture of materials, and subsequently assigns a suitable single representative structure from that mixture to use in all further calculations. In summary, in order to use predictive methods on commercial products such as PCBs, or when capturing or querying information in structure- searchable databases for these types of mixtures, the developers must employ scientific judgment to select suitable, discrete structures to represent chemical mixtures in their tools.

For complex commercial products such as PCBs, often represented by a single CAS number, many scientifically acceptable representative structures can be used in an assessment and the corresponding measured data relating to these chosen representative structures will vary slightly depending on the particular molecule chosen to represent the mixture. These slight variations in assessment values noted between tools do not reflect errors in the predictions or databases, but rather reflect differences in the structures chosen by the scientific development staff. To further clarify, there is currently no harmonized, universal set of procedures or lists of structures for choosing standard representative molecules for each commercial product, isomeric mixtures, or lists of CAS numbers in the scientific community. Inevitably, variations in decision points will occur and it is not uncommon for these small variances to be observed when reviewing multiple databases, or when making quantitative predictions, particularly when the estimates are based on CAS number as the input data.

EPI Suite ™ integrates available science and is easy to use, transparent, and cost-effective. At the request of the EPA's Office of Pollution Prevention and Toxics (OPPT), EPA's independent Science Advisory Board (SAB) reviewed EPI Suite™ (of which KOWWIN is a component). Upon receipt of the SAB final report, the Agency will evaluate the recommendations to determine the appropriate actions to be taken. Additional information can be found at the SAB Estimation Programs Interface (EPI) Suite Review Panel Web Site.[1] The Agency plans to undertake enhancements to EPI Suite™ in areas related to data quality, transparency and uncertainty. Once these activities have been completed, the Agency plans to update other tools, such as the PBT Profiler, accordingly, as funds are available and to the extent that the EPI Suite™ software upgrades apply. More detail on the planned work is given below under Actions Taken.

**Actions Taken:**

- The reference database CHEMFATE has been edited to now provide a ***range*** of log Kow values from 4.53 to 8.3 (mono- to decachlorobiphenyl) for CAS 1336-36-3, without recommending any particular value. This range is based on experimental data from Hansch et al. (1995). Reporting or retrieving data as a range of values can be done for CHEMFATE, as this database simply provides raw data to the user, but ranges can not be recorded in other tools such as EPI Suite™ and PBT Profiler, as these methods need a single structure or reference point as input to further manipulate the data and to make predictions for an array of environmental endpoints.

- The Agency is looking into updating EPI Suite™ and its component programs including KOWWIN to more clearly describe how it treats mixtures such as those represented by PCB CAS numbers 1336-36-3 and 11097-69-1. This methodology is already fully described in the PBT Profiler online documentation.

- The Agency is working to increase the transparency of data variability and uncertainty in EPI Suite™ (KOWWIN). Our plans are to provide information in a consistent way in the program Help files and to include a confidence interval associated with estimated property values derived from that program. For each program like KOWWIN, we plan to provide this information in a separate paragraph that contains model statistics such as mean error and coefficient of determination. We expect each Help file to address in a general way error associated with the experimental data in the model's training set. On validation, the Agency intends to update and enhance information in EPI Suite™ Help files so that for each program validation is addressed explicitly, including relevant studies published since development of the models. Transparency will also be enhanced in a variety of other ways. These enhancements are not specific to KOWWIN; nonetheless they may be applicable to software such as the PBT Profiler. Examples include validation of the SMILECAS file; inclusion of full

[1] Science Advisory Board Estimation Programs Interface (EPI) Suite Review Panel Web site - http://www.epa.gov/sab/panels/epi_suite_review_panel.htm

reference citations for all experimental data within EPI Suite's ™ several internal data files (one of which is PhysProp); inclusion in each EPI Suite™ Help file of a separate section on temperature dependence of the property; and expression of model output using the International System of Units (SI).

**Chamber Request:** Ensure the correctness of databases and models that are owned by a third-party.

**EPA Response:** When EPA provides funding for database development, the Agency generally does not determine the content and presentation of information on privately-owned Web sites. Two of the databases identified by the Chamber, PhysProp and CHEMFATE, are owned by SRC. EPA asked SRC to make improvements to the PhysProp and CHEMFATE databases pursuant to an existing contract between EPA and SRC. These improvements will make the information in these databases more consistent with the EPA IQG. The Agency provides links to these Web sites, not as an endorsement of the information, but rather as a convenient tool to provide users with additional information. Links to external information on EPA Web sites include a notification that external sources do not represent Agency policy or information.[2]

**Actions Taken:**

- EPA conveyed the Chamber's concerns about transparency to SRC, the proprietary owner of PhysProp and CHEMFATE. In response, SRC made available online their multi-step internal review process in the Environmental Fate Data Base (EFDB) Web site[3] and in the SRC PhysProp Web site.[4] SRC now provides references to the articles describing methodology, as well as details of the review process.

**Chamber Request:** Evaluate EPA's use of Web site notifications.

**EPA Response:** EPA believes that the databases and tools identified in the Chamber's RFR are transparent regarding the sources and utility of the data. EPA recognizes, however, that there has been less transparency regarding the review processes to which the databases have been subjected. Since receipt of the RFR, EPA has taken action to clarify these processes and the Web site notification language in the databases. The use of such notifications is a well-established government and industry practice that serves the purpose of notifying users of the quality and limitation of information. Generally, such statements provide users with disclosures of the specific data sources that have been used and the specific quantitative methods and assumptions that have been employed.

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[2] EPA External Site Links Procedure, September 7, 2006, http://yosemite.epa.gov/OEI/webguide.nsf/standards-guidance/external-links

[3] Environmental Fate Data Base (EFDB): http://www.syrres.com/Esc/efdb.htm

[4] The Physical Properties Database (PHYSPROP): http://www.syrres.com/esc/physprop.htm

**Actions Taken:**

- EPA revised the opening screen Web site notification in the EPI Suite™ (which contains KOWWIN™), further clarifying the intent and purpose of the software.[5]

- EPA updated the notification language for WATER9 to reflect standard language consistent with other EPA software and databases.[6]

- EPA has updated the EPI Suite™ User Guide to include new sections about Limitations and Data Quality Considerations which discuss the appropriate use of EPI Suite™.

- EPA updated Web site notification language for its exposure assessment tools and models.[7]

[5] Estimation Program Interface (EPI) Suite™: http://www.epa.gov/opptintr/exposure/pubs/episuite.htm
[6] WATER9, Version 2.0, Released July 1, 2004, http://www.epa.gov/ttn/chief/software/water/index.html.
[7] Exposure Tools and Models Web site, http://www.epa.gov/oppt/exposure/pubs/fqa.htm#envfate and http://www.epa.gov/oppt/exposure/pubs/fqa.htm.

## Appendix B: IQG Attributes

EPA maximizes the quality of information found in its disseminated databases and models by ensuring that the objectivity, utility, integrity, and transparency of the information is adequate for its intended use. "Objectivity" focuses on whether the disseminated information is being presented in an accurate, clear, complete, and unbiased manner, and as a matter of substance, is accurate, reliable, and unbiased. "Utility" refers to the usefulness of the information to the intended users. "Integrity" refers to security, such as the protection of information from unauthorized access or revision, to ensure that the information is not compromised through corruption or falsification. "Transparency" involves the provision of information to the user regarding data sources, methods, and other aspects of data quality. This description of objectivity, utility, integrity, and transparency is consistent with the Office of Management and Budget (OMB) Guidelines for Ensuring and Maximizing the Quality, Objectivity, Utility, and Integrity of Information Disseminated by Federal Agencies[1] (OMB's IQGs), and EPA's Guidelines for Ensuring and Maximizing the Quality, Objectivity, Utility, and Integrity of Information Disseminated by the Environmental Protection Agency[2] (EPA's IQGs).

The Chamber identified sixteen sources of information. These include five databases, one user interface, four documents and six models[3]. As noted in our RFC response, three of the models (CHEMDAT8, CHEM9, SIMS), the user interface (SCDM Win) and one of these documents (SPHEM) were superseded. One database (STF) was removed from the EPA Web Site. One database could not be identified. In its RFR, the Chamber identified this database as the "Handbook of RCRA Ground-water Monitoring Constituents: Chemical & Physical Properties."[4] In regard to the issues raised by the Chamber, this document does not include a Log $K_{ow}$ value for "Polychlorinated biphenyls; PCBs; Aroclors."[5]

The following tables describe the attributes that contribute to the objectivity, utility, integrity, and transparency of the remaining eight models, databases and documents identified in the Chamber's RFR.

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[1] 67 Fed. Reg. 8452 (February 22, 2002). http://www.whitehouse.gov/omb/fedreg/reproducible2.pdf

[2] 67 Fed. Reg. 63657 (October 15, 2002)
http://www.epa.gov/quality/informationguidelines/documents/EPA_InfoQualityGuidelines.pdf

[3] **Databases**: SCDM, STF, TreatDB, PhysProp, CHEMFATE **User Interface:** SCDM Win **Models**: CHEMDAT8, SIMS, CHEM9, KOWWIN, WATER9, PBT Profiler **Documents:** RCRA, SPHEM, HHRAP, HHRAPCF

[4] Handbook of RCRA Ground-Water Monitoring Constituents: Chemical and Physical Properties (40 CFR Part 264, Appendix IX), EPA, 1992,

[5] In this document, the log $K_{ow}$ value for Polychlorinated biphenyls; PCBs; Aroclors is listed as "NA."

| HHRAP | |
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| DESCRIPTION | • The 1998 peer review draft of the Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities (HHRAP)[6] was superseded by the 2005 version. This guidance document provides a user-friendly approach to performing site-specific human health risk assessments of hazardous waste combustors.<br>• This version includes *The Hazardous Waste Companion Database* that updates and replaces the hard-copy listing of chemical-specific parameter values originally found in Appendix A of the 1998 HHRAP. |
| USE | • The Companion Database is a one-stop source for the chemical-specific property values for anyone using the HHRAP to perform a screening level site-specific human health risk assessment of a hazardous waste combustor. |
| ATTRIBUTES | • The Companion Database addresses comments received from the public and external scientific peer reviewers regarding chemical-specific parameter values found in earlier drafts of the HHRAP.<br>• HHRAP Appendix A-2 details the hierarchy of sources for, or equations used to calculate, parameter values found in the Companion Database. The Companion Database includes citations for individual parameter values.<br>• All users must accept the Companion Database Initial Agreement before they can access the database. This agreement contains detailed notifications regarding the appropriate uses and limitations of the data found in the database.<br>• EPA intends to post periodic updates to the Hazardous Waste Companion Database on the web site - http://www.epa.gov/epaoswer/hazwaste/combust/risk.htm to ensure that the information maintained in the database is current.<br>• Both the HHRAP and the Companion Database refer the user to the email account, "HHRAPFeedback@epa.gov", a central clearinghouse for questions/comments, including suggested changes to parameter values listed in the Companion Database. |

| KOWWIN™ | |
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| DESCRIPTION | • KOWWIN™ is a model that estimates the log octanol-water partition coefficient (log $K_{ow}$) of chemicals using an atom/fragment contribution method. This model is one of the components of the EPA Office of Pollution Prevention and Toxics (OPPT's) Estimation Programs Interface (EPI) Suite™ – a suite of physical/chemical property and fate estimation models.<br>• The model was developed by Syracuse Research Corporation (SRC). |
| USE | • The model provides users with screening level estimations of physical/chemical properties and environmental fate properties. KOWWIN estimation is considered to have acceptable accuracy for screening-level assessments for most discrete organics. |

[6] Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities (HHRAP), EPA, 2005. http://www.epa.gov/epaoswer/hazwaste/combust/risk.htm

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| ATTRIBUTES | • The KOWWIN Program methodology is described in the following peer-reviewed journal article: Meylan WM, Howard PH. 1995. *Atom/fragment contribution method for estimating octanol-water partition coefficients*. J. Pharm. Sci. 84:83-92. The citation for this article is given in EPI Suite™.<br>• Information on SRC's peer review process for log $K_{ow}$ data in KOWWIN is also given in the J. Pharm. Sci. publication cited above.<br>• Data are derived from calculation (via the KOWWIN estimation method) and a linked file of measured values from the peer-reviewed scientific literature (e.g. Hansch et al. 1995).<br>• During development by SRC, the model was subjected to a multi-step peer-review process.<br>• Measured values are selected after a multi-step review by SRC.<br>• Data are subjected to constant reviews by developers and users.<br>• References are provided for experimental $K_{ow}$ values, allowing the user to assess the utility of values derived from log $K_{ow}$ estimation method and validate the results.<br>• Estimated KOWWIN™ results are derived from a standard estimation methodology contained within the KOWWIN™ program. Data used to develop and validate the estimation method are available in KOWWIN™.<br>• The EPI Suite™ model provides information on the appropriate uses of KOWWIN™.<br>• The USEPA Science Advisory Board (SAB) EPI Suite Review Panel reviewed OPPT's EPI Suite™ Software at a public meeting March 7-9, 2006. The panel is in the process of finalizing its report which will subsequently be reviewed by the chartered board.<br>• Experimental KOWWIN™ data are embedded within the EPI Suite™ software, and cannot be accessed until the user downloads it. The database data cannot be altered.<br>• EPI Suite™ can only be downloaded from EPA's Web site.<br>• Training on EPI Suite™ was delivered during OPPT's Sustainable Futures project. |

| **PBT Profiler** | |
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| DESCRIPTION | • PBT Profiler is an online screening tool for estimating persistence, bioaccumulation, and toxicity (PBT) potential of individual chemical compounds.<br>• PBT Profiler was developed by SRC for EPA OPPT.<br>• PBT Profiler uses "measured" values for total PCBs and Aroclor 1254. |
| USE | • The screening tool is made available to industry and other stakeholders for use in setting priorities early in research and development.<br>• This tool also helps set priorities for focusing resources. |
| ATTRIBUTES | • PBT Profiler was subjected to extensive pre-dissemination review and beta testing by industry, academia, and governmental institutions.<br>• Peer review was conducted in accordance with EPA's Peer Review Policy. Complete information regarding the peer review of the PBT Profiler is available at www.regulations.gov, click on "Advanced Search" and search for Docket ID: EPA-HQ-OPPT-2002-0025 or Title: "PBT Profiler Peer Review." |

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| | • The PBT Profiler Web site contains detailed notifications regarding the appropriate uses and limitations of the PBT Profiler.<br>• Information on the specific model components of the PBT Profiler can be accessed by down loading and installing the integrated set of models from EPI Suite™ [7] at no cost.<br>• The PBT Profiler does not provide direct access to the underlying PBT Profiler databases and methodology. |

| SCDM | |
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| DESCRIPTION | • The Superfund Chemical Data Matrix (SCDM) (http://www.epa.gov/superfund/sites/npl/hrsres/tools/scdm.htm) compiles data on physical, chemical and toxicological properties of hazardous substances from other EPA-developed literature sources and databases, and/or peer reviewed literature sources and databases. It does not generate chemical data but merely "borrows" data from these other sources.<br>• The SCDM was developed by the EPA Office of Solid Waste and Emergency Response (OSWER) for use by EPA staff and other individuals involved in implementing the Hazard Ranking System. |
| USE | • The SCDM is only intended to be used when applying the Hazard Ranking System (HRS) to potential National Priorities List (NPL) sites. It compiles various useful data on hazardous substances in a "one-stop" easy-to-use reference. |
| ATTRIBUTES | • Data are drawn from peer-reviewed scientific literature, EPA-developed literature, and databases such as PhysProp and CHEMFATE.<br>• Each data field populated in SCDM references the original data source.<br>• EPA scientists reviewed the data sources to verify the appropriateness of their inclusion in SCDM.<br>• When there are several sources available for a certain data type, SCDM provides a hierarchy (listed in order of preference) of the data sources used to assign a single value into SCDM.<br>• Detailed information regarding the processes and procedures through which the values contained in the SCDM were derived and the sources from which the input data were obtained are provided in the Data Selection Methodology chapter of the "*Superfund Chemical Data Matrix Methodology*" [8] (http://www.epa.gov/superfund/sites/npl/hrsres/tools/method_2.pdf).<br>• SCDM values are documented in the HRS documentation record for each site proposed to the NPL, in a proposed rule in the Federal Register. The HRS documentation record is available for public review and the public has 60 days to provide comments on EPA's HRS evaluation of the site including the SCDM values. |

[7] Estimation Program Interface (EPI) Suite™: http://www.epa.gov/opptintr/exposure/pubs/episuite.htm

[8] *Superfund Chemical Data Matrix Methodology*, EPA Office of Solid Waste and Emergency Response, January 2004. (http://www.epa.gov/superfund/sites/npl/hrsres/tools/scdm.htm )

| TREAT DB | |
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| DESCRIPTION | • Treatability Database, Version 5.0, 1994, http://www.epa.gov/ORD/NRMRL/treat.htm is a CD compilation provided by the EPA National Risk Management Research Laboratory (NRMRL) that summarizes the treatment technologies used to treat a specific chemical; the type of waste/wastewater treated; the size of the study/plant; and the treatment efficiency achieved.<br>• TREAT DB contains 1,217 chemical compounds and over 15,800 sets of treatability data. For each chemical, the database includes: physical/chemical properties (molecular weight, boiling point, melting point, etc.), aqueous and solid treatability data, and Freundlich isotherm data. |
| USE | • The database is primarily used as a ready literature review of treatment efficiencies that can be expected for a wide variety of technologies and matrices.<br>• The Treat DB compilation supports EPA, States, and Industry review of potential treatment strategies. |
| ATTRIBUTES | • Data are drawn from existing sources that are cited with full documentation in the database.<br>• Thorough reviews of data entries and data quality were made prior to entry into the database.<br>• For each chemical, the database documents other environmental database information sources, and data references with a reference abstract.<br>• Each data set is also referenced to sources of information, operational information on process(es) sampled and quality coded based upon analytical methods and reported quality assurance. |

| WATER9 | |
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| DESCRIPTION | • WATER9 is a wastewater treatment model. This windows based program calculates organic air emissions from wastewater collection and treatment and other waste treatment operations. |
| USE | • The model helps regulated communities determine air emissions from their facilities. This model also helps EPA, States and industry in developing air emissions reduction programs. |
| ATTRIBUTES | • Documentation regarding collaborative work with industry regarding WATER9's chemical properties database is available from OAQPS upon request.<br>• Data are drawn from peer-reviewed scientific literature, widely used databases, and precursor models and databases.<br>• Emission models are literature models that were developed and published by university researchers.<br>• WATER9 compiles multiple values of Henry's Law constants found in literature and selects an appropriate value.<br>• Model Database was developed with active involvement by stakeholders.<br>• Prior to its release, WATER9 was subjected to significant peer review and beta testing.<br>• While WATER9 has the capability of using the UNIquac Functional-group Activity Coefficient (UNIFAC) estimation methodology model |

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| | to calculate HLCs, this is not the default. An appropriate value is selected from published values that are widely accepted by EPA and its stakeholders.<br>• Substantial documentation and guidance regarding the installation and use of WATER9 is available at the OAQPS Web site (http://www.epa.gov/ttn/chief/software/water/).<br>• WATER9 data are provided with the model; the user can alter values only after download. |

| PhysProp | |
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| DESCRIPTION | • The Physical Properties (PhysProp) database contains chemical structures, names and physical properties for over 40,000 chemicals.<br>• PhysProp was developed by and is owned by Syracuse Research Corp (SRC) (http://www.syrres.com/esc/physprop.htm).<br>• There are two versions of PhysProp. One is available through the PhysProp Web site maintained by SRC; the other is an integral part of OPPT's EPI Suite™. The SRC version has measured and estimated data from EPI Suite™. The EPI Suite™ version only has measured values. |
| USE | • The database is provided by EPA as a screening tool to help set priorities for risk assessments.<br>• The database enables scientists to identify and retrieve data for assessing exposure. |
| ATTRIBUTES | • During development, the database was subjected to a multi-step peer-review process.<br>• Information about SRC's multi-step internal review process is available online at the SRC PhysProp (Interactive Online Demo version) Web site. (This information was added in response to the Chamber's RFR.)<br>• The PhysProp (SRC) Web site includes a notification to users that the free on-line demo version of PhysProp only retrieves basic data for individual compounds.<br>• Partial reference citations are provided for outputs in both versions of PhysProp, but full reference citations can be obtained through additional literature searches on the Environmental Fate Database (EFDB) Web site.<br>• The on-line version of PhysProp does not provide direct access to PhysProp data.<br>• PhysProp data included in EPI Suite™ are embedded within the EPI Suite software, and cannot be accessed until the user downloads it. The database cannot be altered. |

| CHEMFATE | |
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| DESCRIPTION | • CHEMFATE is a data value file containing 25 categories of environmental fate and physical/chemical property information on important chemical compounds.<br>• Data file was developed by and is owned by Syracuse Research Corp (SRC) (http://www.syrres.com/esc/efdb.htm). |

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| USE | • CHEMFATE enables scientists to find chemical and environmental fate property data without having to search the primary literature. |
| ATTRIBUTES | • Data comes from sources with established evaluation protocols (e.g. Hansch et al 1995; AQUASOL).<br>• Data are drawn from peer-reviewed scientific literature.<br>• Descriptions of the methodology and approach used to develop the data file are available in several peer reviewed articles.<br>• During development, the data file was subjected to a multi-step peer-review process.<br>• SRC uses a multi-step internal review process to control the quality of the data contained in CHEMFATE. When appropriate, data are updated.<br>• Information about SRC's multi-step internal review process is available online at the EFDB Web site. References to the articles describing the SRC methodology are given, as well as details about the review process.<br>• CHEMFATE output includes a full set of references for each of the values provided. This allows users to validate the results and assess the utility of the information for their intended use.<br>• The CHEMFATE Web site does not provide direct access to CHEMFATE data. |