Final Report:
Part 201: Updating Chemical–physical Parameters and Toxicity Data

August 2014

Prepared for
The Criteria Stakeholder Advisory Group (CSA)

Submitted by
TAG 1: Chemical-physical Parameters and Toxicity Data

In collaboration with
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Introduction

Technical Advisory Group 1 (TAG) met six times in June and July 2014 to review, discuss, and develop responses and recommendations related to nine questions that were outlined in the White Paper prepared by Public Sector Consultants Inc. (PSC) addressing chemical–physical parameters and toxicity data used to derive Part 201 generic criteria.[1] PSCs' White Paper served as the framework for the TAG's discussions. This final report to the Criteria Stakeholder Advisory Group (CSA) presents the TAG's discussions, findings, and recommendations.

WHITE PAPER AND REVIEW PROCESS

Overall, the group's impression of the White Paper was positive. Members reported that it is well designed, and that it provided sufficient guidance to the group on where members should be focused. However, the group requested insertion of a brief explanation at the beginning of the White Paper on this project and the Michigan Department of Environmental Quality's (MDEQ) goal of updating the Part 201 rules. As a result, PSC proposed the following language be inserted into the White Paper:

"The Cleanup Criteria Rules are authorized pursuant to Part 201, Environmental Remediation, of the Natural Resources and Environmental Protection Act (NREPA), 1994 PA 451, as amended (MCL 324.101 to 324.90106). The 2010 amendments (2010 PA 228) to Part 201 included the requirement for the Michigan Department of Environmental Quality (MDEQ), to evaluate and revise the cleanup criteria, and incorporate knowledge gained through research and studies in the areas of fate and transport and risk assessment. The MDEQ shall also take into account best practices from other states, reasonable and realistic conditions, and sound science, as required by Section 20120a(18) of NREPA. To that end, the MDEQ has established a Criteria Stakeholder Advisory Group (CSA) to provide input for the process. The CSA consists of professionals from academia, the private sector, and nongovernmental organizations.

The workgroup is charged to review the existing rules, and determine if the criteria should be updated. If the workgroup supports updating the criteria, the charge will be to:

- Identify guiding principles to be used as the basis for updating the criteria;
- Apply the guiding principles in the selection of assumptions to be used in updating the criteria; and
- Provide recommendations to the director of the MDEQ for updating the toxicological and physical chemistry aspects of the cleanup criteria rules."

When TAG members reviewed the nine questions formulated by the CSA and presented in the White Paper, they suggested a realignment for several questions and a clarification on one. Specifically, the group recommended looking at Question 1 and 5 together, and similarly grouping Questions 2 and 4 and Questions 4 and 6, and seeking clarification on Question 7.

This report is organized with each White Paper question posed, the background discussion, and the resulting recommendations.

[1] White Paper: Chemical–physical Parameters and Toxicity Data, Public Sector Consultants, May 2014.

TECHNICAL ADVISORY GROUP MEMBERS

Exhibit 1 details the TAG membership:

EXHIBIT 1. TAG Members

John Buchweitz, PhD, DABT	Michigan State University
Steve Crider, MS	Barr Engineering Co.
Jennifer Gray, PhD	Michigan Department of Community Health
Betty Locey, PhD, DABT	ARCADIS
Eric Wildfang, PhD	Michigan Department of Environmental Quality
Lisa Yost, MS, DABT	ENVIRON Corporation

WHITE PAPER QUESTIONS

The TAG was asked to review and address the following questions and issues:

1. Is the process utilized by the MDEQ since 2002 to select chemical-specific values including toxicity values and physical chemistry parameters appropriate? If not, what should be changed?
2. Have the most robust and reputable data sources been selected to generate the data needed to establish the numeric values under Part 201 rules, or are there alternative databases that should be used?
3. What recommendations should be considered for updating the chemical-specific values, given the directive to use best practices, reasonable and realistic conditions, and sound science? How do these terms relate to changes in toxicity data and chemical–physical parameters?
4. What minimum set of standards, if any, should define acceptable data sources?
5. Should a hierarchy of data sources be established? If not, please provide a rationale. If so, what should the hierarchy of sources be, and are there any circumstances under which deviations from the hierarchy should be allowed?
6. Can the Technical Advisory Group provide a descriptive level of quality that could be used as a framework for selecting data sources?
7. Should the MDEQ-derived "toxicity values" be consistent with or based upon federal (i.e., U.S. Environmental Protection Agency (EPA)) methodology and data? If so, are there any circumstances under which deviations from the federal (i.e., EPA) methodology and data should be allowed?
8. Should an independent evaluation of the chemical-specific data be conducted even if a value is published in the primary database of the hierarchy?
9. For chemical–physical parameters, should experimentally-derived estimates take precedence over theoretically-derived estimates?

SUMMARY OF TAG RECOMMENDATIONS

A subset of toxicity values and some chemical–physical parameters promulgated in Part 201 are outdated. In general, the TAG recommendations define a framework that allows for the identification of toxicity values and chemical–physical parameters that represent the best available science, best practices (from U.S. Environmental Protection Agency, other federal agencies, and other states and countries), reasonable and realistic conditions, and sound science, as required by Section 20120a(18) of the Natural Resources

and Environmental Protection Act. Recommendations also include flexibility for program changes within a reasonable time frame as the science evolves, and ways to increase transparency in the process.

The TAG identified a list of acceptable sources for chemical–physical parameters and toxicity values and proposed two decision frameworks (see Appendices A and B). An alternative to the framework in Appendix A was proposed by a member who believes that EPA's Soil Screening Guidance (SSG) recommendations for the selection of most chemical–physical parameters are still more robust and scientifically sound than any other subsequent EPA guidance. The rationale this TAG member provided and the responses to comments from other members who oppose using SSG as the primary source are included in Appendix E.

For the decision frameworks a tiered list of reference sources for toxicity values is included for consideration by the CSA. In addition, the TAG recommends that additional referencing be added to MDEQ Table 4—Toxicological and Chemical-Physical Data: Part 201 Generic Cleanup Criteria and Screening Levels—and that the basis for each value be provided on the MDEQ's website for interested users.

A process and timeline for the MDEQ to update the December 2013 version of Table 4 and the resulting Part 201 Generic Cleanup Criteria and Screening Levels was developed by the TAG (Appendix C). It would to allow for an open submission period (e.g., three years) and a petition process for chemicals to be considered for update in Years 1, 2 and 3 based on availability of relevant new scientific information. In Year 3, the MDEQ would identify which chemicals would be updated based upon available information; in Year 4, the department would allow a comment period and then move through the legislative rule process (the question of how updates will be structured in a legal context is being examined by TAG 4 – Legal). Also proposed is a new chemical update worksheet to assist in updating chemical–physical parameters and toxicity data (Appendix D).

The TAG definition of "update" for purposes of TAG 1 discussions was limited to chemical–physical values and toxicity values and resulting criteria, not equations themselves or exposure inputs, which were beyond the scope of this group. The TAG understands that other areas of the Part 201 cleanup criteria rules are currently under review by the other TAGs and may result in additional considerations as to how criteria "updates" are ultimately defined by the CSA. For the purposes of TAG 1, the "four year update cycle" was developed and is presented in the context of reviewing the chemical-physical and toxicological data to determine if the current values represent the best available data.

A total of twelve recommendations are offered for the CSA's consideration.

Questions, Answers, and Recommendations

The following section presents each White Paper question, a summary of the TAG's discussion, and recommendations. Note that several questions were realigned by the TAG consistent with the information being discussed and the overlap among topics. This report organizes the questions as they were considered and addressed by the TAG.

Question 1

Is the process utilized by the MDEQ since 2002 to select chemical-specific values including toxicity values and physical chemistry parameters appropriate? If not, what should be changed?

Summary Answer: Yes, but there is opportunity for improvement. The TAG agrees with the MDEQ and other practitioners that many of the chemical-physical parameters and toxicity values currently promulgated in Part 201 should be updated, as appropriate, to be consistent with the best available science, and that a process should be established for periodic updates to these values to insure that they continue to be based on the best available science. The TAG developed and recommends two new decision frameworks to update toxicity values and chemical–physical parameters (Appendices A and B) underpinned with transparency and best available science. An alternative view provided by a TAG member for updating chemical–physical parameters is also outlined in Appendix E.

Recommendation 1: The MDEQ should adopt the decision-making frameworks as proposed**.** As indicated above and highlighted throughout the discussion sections of this document, an alternative view emerged for prioritizing EPA's SSG recommendations for the selection of chemical–physical values.

Recommendation 2: The MDEQ should include a short reference for each value and chemical-physical parameter in Table 4 that identifies the source of the values and that also indicates whether physical parameters are measured or modeled when relevant. A more detailed explanation of the reference could be stored in a separate table or other resource as this would give each value greater transparency. A similar model is being used by the Ontario Ministry of the Environment, Canada, and the MDEQ should consider this format while designing its updated tables.

Recommendation 3: The MDEQ should provide more opportunity for stakeholders to give feedback on what data and methodology could be considered in selecting parameters or developing toxicity values when the MDEQ determines it is necessary to develop such values.

Recommendation 4: When administrative rules are updated, the inhalation toxicity terms in the VSIC, PSIC, GVIIC, and SVIIC equations and relevant rule language should be changed to allow the MDEQ the flexibility to select inhalation toxicity values that differ from those developed by the MDEQ's Air Quality Division (AQD), considering best available science and practices. The MDEQ's Remediation and Redevelopment Division (RRD) staff should not have to evaluate all inhalation toxicity values, though some attention should be given to those that are based upon the AQD's most minimal data requirements at the time they are evaluated. Inhalation toxicity value reference sources should be included in Table 4.

Discussion

The TAG discussed the MDEQ's legislative mandate to update its process for selecting chemical–physical parameters and toxicity values, and concurs that the process should be made easier to update, occur more frequently, be more transparent, incorporate the best science available, and allow for professional judgment. The issue of using the best available science and allowing for professional judgment in the process are included in the discussion on developing a tiered list of reference sources in Question 5 below.

Physical–chemical Parameters

In considering physical chemistry parameters, the group acknowledged the underlying issue of deciding whether the process should rely more on model-based values or on experimentally values. There was agreement within the TAG that experimentally-derived (measured) values are preferred, so long as the methods used in the experiment are clearly presented and are carried out at acceptable temperature and pressure. However, there was disagreement on how to select a value from among multiple valid measured values when these values differ significantly. This disagreement ultimately concluded in two different perspectives on how and where EPA's SSG recommendations on chemical–physical parameters should be used in a decision framework. While the MDEQ seeks to utilize experimental data whenever possible, the department also values consistency and would prefer an updated process to allow for both—especially considering staff resources and the time it takes for these updates to occur. The data source used first by the MDEQ is ChemIDplus: a free, Web-based search system that provides access to the structure and nomenclature authority files used for the identification of chemical substances cited in National Library of Medicine (NLM) databases—including the TOXNET® system. ChemIDplus also has structure searching and direct links to resources at NLM, federal agencies, U.S states, and scientific sites. The database contains more than 400,000 chemical records, of which more than 300,000 include chemical structures.

ChemIDplus reports both experimental data and estimates derived through modeling. One concern with model approaches is that they can derive estimates outside the range of experimental values, resulting in an inaccurate representation of the chemical's behavior for the criteria calculations.

At least one TAG member suggested that the default chemical–physical parameter values should continue to be based on the U.S. Environmental Protection Agency's (EPA) recommendations from the SSG, with allowance for parameter-specific deviations where scientifically justified. Discussion on the rationale for MDEQ's existing use of EPA's SSG recommendations and examples of why at least one TAG member believes the SSG approach is technically sound and superior to values from EPI Suite and ChemIDPlus are included in Appendix E.

Toxicity Values

When updating toxicity values, the MDEQ's preference is to utilize best available science and research. The department recognizes that members of the regulated industry can help provide this information and play a valuable role. Allowing for more public comment is another way to improve the transparency of the process. For example, the MDEQ's Air Quality Division (AQD) announces a short list of chemicals to be updated each month and seeks public input on these chemicals for a specific time period before updating the value. Additionally, the EPA Scientific Advisory Board recently released recommendations for process improvements to EPA's Integrated Risk Information System (IRIS). This document was available to TAG members and the group considered these recommendations when developing a new update process for the MDEQ.

The group also reviewed the MDEQ AQD's air control rules, which are currently being updated. A TAG member indicated there is a new procedure proposed to create the initial list, change a value, or to add or delete a chemical from the list. Group members indicated that Initial Threshold Screening Levels (ITSLs) and Inhalation Unit Risk Factors (IURFs) are values that are developed by the AQD that are used to calculate the Part 201 volatile soil inhalation criteria (VSIC), particulate soil inhalation criteria (PSIC), groundwater volatilization indoor air inhalation criteria (GVIIC), and soil volatilization indoor air inhalation criteria (SVIIC). The equations, as currently presented in the Part 201 administrative rules, use these exact terms, ITSL and IURF. MDEQ's RRD uses these AQD values to calculate inhalation-based criteria.

Historically, an effort has been made by the MDEQ to identify peer-reviewed data sources populated with information developed using the best available science and consistent with the most current subject matter

guidance. Preference was given to extensive and robust data sources having high credibility in the relevant scientific community. Both the data sources and the information on chemical-specific parameters have changed over the years. The documentation for sources of information used in the past was not routinely recorded and, in some cases, information on the source(s) used is simply not available today. The MDEQ has received recommendations in the past with respect to documenting the priority given to the use of a variety of available data sources.

Topics explored by the TAG include:

- **Rules vs. statute:** Is it better to have a revised Table 4 promulgated in rules, or included in statute? Members decided to let TAG 4 (Legal) explore the best approach (i.e., statute vs. rules, grandfather clause).
- **Timing of *updates*:** The toxicological, chemical, and physical parameters utilized by the MDEQ to calculate the cleanup criteria are currently promulgated as rules and can be found in Table 4 of R 299.50. Table 4 has not been fully updated since 2002. A TAG member indicated that the legislature and business community would support predictable updates, and agreement emerged among group members that it should occur more frequently. One challenge identified by the MDEQ is that the agency has struggled with what satisfies the definition of *update*. For purposes of this discussion, the TAG definition of *update* is limited to chemical–physical values and toxicity values and resulting criteria versus equations themselves.
- **Process for Updating Chemical–Physical and Toxicological Data**: A proposal for the MDEQ to update Table 4 every four years emerged from the TAG (Appendix C). It would to allow for an open submission period (e.g., three years) and a petition process for chemicals to be considered for update in Years 1, 2, and 3 based on new or previously unavailable, relevant scientific information. In Year 3, the MDEQ would identify which chemicals would be updated, based upon available information; in Year 4, the department would allow a comment period and then move through the legislative rule process (if necessary). It was noted that the MDEQ has internally discussed annually posting candidates (e.g., five to ten chemicals a year that need to be re-evaluated). The candidate chemicals would come from an open submission period, a petition process for chemicals to be considered, and updated toxicity values that come through IRIS or other significant sources.

Question 5

Should a hierarchy of data sources be established? If not, please provide a rationale. If so, what should the hierarchy of sources be and are there any circumstances under which deviations from the hierarchy should be allowed?

Summary Answer: The MDEQ should use a tiered approach (Recommendation 1) that replaces the term *hierarchy* with the term *decision framework*. Transparency and flexibility are built into the decision frameworks.

Recommendation 5: The MDEQ should adopt the two proposed decision frameworks (Appendices A and B that loop back to best science and allows for professional judgment). See Appendix E for alternative view.

Recommendation 6: The MDEQ should utilize the chemical update worksheet (Appendix D) to collect information and as a communication tool—a Web-friendly version (i.e., a PDF) should be placed on MDEQ's website.

Discussion

The group reviewed the MDEQ data source hierarchy provided in the White Paper. The TAG agreed that, to be transparent and consistent in the process for determining the chemical–physical and/or toxicity

parameters, it is essential to have a process that utilizes specific data sources. However, it agreed that the term *hierarchy* should be replaced with the term *decision framework*, using a tiered approach to more accurately reflect the proposed process chart. Additionally, a decision framework will allow for those outside of the MDEQ to arrive at (or duplicate) the same value as the department, while recognizing, however, that professional judgment and interpretation may not always allow for the precise replication of results.

The variability of model-based versus experimentally-derived values was discussed. To evaluate the impact of the proposed changes in sources of chemical–physical and toxicological data, the group examined the variability, or relative percentage difference, between the Framework-derived values and the current values (from MDEQ Table 4). A member had analyzed the percentage differences between current toxicity and chemical–physical values (from MDEQ Table 4) and those derived using the decision framework, and some large numerical differences (both negative and positive) appeared to exist. It was noted that some errors exist in the current Table 4 values but, since they are promulgated currently, little can be done to update them at this time. However, no analysis has been performed to determine the effect of the proposed toxicity value and chemical–physical value changes (either separately or combined) on the existing Part 201 criteria.

The group discussed the percentage differences and considered whether there is a certain level of variance that warrants further investigation and/or whether there is a subset of major chemicals with any level of variability that warrants further investigation. Additionally, the TAG considered what other criteria need to be used—besides the age of the data source—when moving away from the decision framework, and determining when best professional judgment is acceptable. While no conclusions or recommendations resulted from these discussions, members found the information valuable—which helped inform broader discussions. The TAG emphasized Recommendation 2: linking source information to the tables, and providing information on whether the data are experimental or modeled—which could be a valuable tool during the criteria update process. (Note to reader: This discussion is also relevant to Question 3).

Chemical–Physical Parameters

Decision frameworks highlighting the proposed steps to update values were developed by a TAG member and are recommended by the group (Appendix B). Members like that the chart clarifies that the MDEQ use experimental data in lieu of modeled data. Members noted that when Table 4 is updated, it should indicate the data sources—including the version of the program—if applicable. One member identified that this proposed approach does not have the ability to choose among multiple valid experimental values and thus recommended that the SSG recommendations currently used in Part 201 continue to be prioritized first because it has successfully addressed this issue. See Appendix E for additional background and discussion.

Toxicity Values

The group noted that, when reviewing a chemical, toxicity values would be evaluated to see which one meets the determination of the best available science. Both peer-reviewed studies and unpublished industry studies that follow good laboratory practices would be acceptable and considered during an evaluation. After discussion of California EPA requirements, some members strongly encourage the MDEQ not to use the California values in situations where California has identified a carcinogen, but that finding has not been embraced or utilized by agencies outside of California.

Question 2

Have the most robust and reputable data sources been selected to generate the data needed to establish the numeric values under Part 201 rules, or are there alternative databases that should be used?

Summary Answer: Since many of the promulgated toxicity values have not been revised since 2002, they may not necessarily be based on the most robust and reputable data sources.

Recommendation 7: Update all values based on a tiered approach as described in response to Questions 1 and 5 above. Recommended resources should be expanded to include international data sources, including, but not limited to, European and Canadian sources.

Discussion

TAG members noted that when data on a chemical is limited there may be unpublished or proprietary references that companies may submit for the MDEQ's consideration, and that default values for certain chemical-specific parameters (such as absorption efficiency and relative source contribution) may be used for chemicals when chemical-specific data is unavailable. Therefore, additional reference sources should be available to the MDEQ to fill data gaps if the data meets the fundamental requirements of an acceptable data source (see Recommendation 8).

The current proposed list of resources for the physical and chemical properties is listed in Chemical-Physical Value Decision Framework (Appendix A) and the current list of resources for toxicity values is included in the Toxicity Value Decision Framework (Appendix B).

Question 4

What data sources should the department consider in conducting these revisions? What minimum set of standards, if any, should define acceptable data sources?

Summary Answer: See Recommendation 8 below.

Recommendation 8: The TAG supported data sources for chemical-physical parameters and toxicity values consistent with the fundamental data source characteristics presented below:

- **Peer-reviewed:** Every effort should be made to identify and use peer-reviewed data sources populated with information that has been developed using the best available science and practices. Scholarly review by experts in the field ensures data meet necessary quality standards prior to publication.
- **Subject to notice and comment:** Toxicity values that are developed by non-MDEQ sources through a process that allows public review and comment are preferred. (Note: It is desirable to allow affected stakeholders [and affected Michigan citizens and regulated community members] input when changing Table 4 values.) In general, chemical-physical data do not undergo public review and comment procedures.
- **Derived through relevant and accepted methods:** Priority should be given to sources that provide chemical-physical and toxicity data based on similar methods as those used for Tier 1 and Tier 2, contain values which are peer reviewed, are available to the public, and are transparent about the methods and processes used to develop the values.
- **Comprehensive:** In the absence of the availability of a single, complete chemical information source for chemical-physical or toxicity data, the MDEQ should utilize data sources that provide the most robust coverage of the Part 201 hazardous substance list. This helps to assure greater consistency of the data used in developing the risk-based values.

- **Credible:** Data sources that are respected and trusted by the international scientific community are preferred.
- **Regularly maintained:** Science evolves. Regular review and updating of the chemical information will assure that it represents the best available science and practices in that field. For example, two recent guidance documents are good resources to consider in selection or development of toxicity values: EPA Framework for Human Health Risk Assessment to Inform Decision Making[2], and National Research Council (2014) Review of EPA's Integrated Risk Information System (IRIS)[3].
- **Based on experimental data:** Chemical data presented in the scientific literature and the many compiled documents and database resources can vary in method of derivation. Experimental chemical-physical data, where relevant to applied environmental conditions, are preferred over extrapolated, modeled, or estimated data. Similarly, experimental toxicity data are preferred, with the understanding that the scientific field is moving away from traditional, whole-animal experimental studies to higher throughput, less resource-intensive in vitro, array, and computer-based toxicity models.

Discussion

The TAG discussed the MDEQ's and the EPA's hazardous substance-specific toxicity and chemical–physical parameter reference sources presented and described in the White Paper. The MDEQ has identified and promulgated numeric values for the chemical-physical parameter and toxicity values required for developing the generic cleanup criteria for most Part 201 hazardous substances. To identify these values, the MDEQ has proposed to establish a preferred list of reference sources based on several fundamental characteristics described initially in the White Paper. Proposed revisions to these characteristics are offered above. Members also suggested using the terms "best available science" or "appropriate studies," rather than "defensible studies."

Question 6

Can the Technical Advisory Group provide a descriptive level of quality that could be used as a framework for selecting data sources?

Summary Answer: Yes. See Recommendations 7 and 8 above.

Discussion

On Question 6 (and Questions 2 and 4), the TAG determined that reputable data sources should be based on the characteristics described Recommendation 8. Specific to Question 6, the group discussed adding to the federal/state databases in the decision framework flow chart. Members recommended not restricting the MDEQ to only the data available today and suggested the flexibility to evaluate future sources in such areas as endocrine disruptor, in vitro, ex vivo, or in silico testing, and shifts in EPA philosophy.

[2] USEPA 2014 available at http://www.epa.gov/raf/files/hhra-framework-final-2014.pdf
[3] NRC 2014 available at http://www.nap.edu/catalog.php?record_id=18764

Question 3

What recommendations should be considered for updating the chemical-specific values, given the directive to use best practices, reasonable and realistic conditions, and sound science? How do these terms relate to changes in toxicity data and chemical–physical parameters?

Summary Answer: Two decision frameworks that propose steps for meeting the requirements for best practices, reasonable and realistic conditions, and sound science were developed and endorsed by the TAG (Appendices A and B). Alternative view is highlighted in Appendix E.

In addition, age-dependent adjustment factors (ADAFs) should be used with toxicity values for those carcinogens identified as mutagenic by the EPA.

Discussion

See the Discussion sections provided under Questions 1 and 5, and Appendices A and B.

In addition, the TAG was asked by TAG 2 to assess the process to determine if a chemical has a mutagenic mode of action and to which substances should age-dependent adjustment factors (ADAF's) be applied (i.e., should Chromium VI be listed as a mutagenic chemical?).

Recommendation 9: Age-dependent adjustment factors (ADAFs) should be used with toxicity values for those carcinogens identified as mutagenic by the EPA or any agency/scientific body as long as it's conducted in accordance with EPA guidelines on identifying mutagenic mode and evaluated by the MDEQ.

Question 7

Should the MDEQ-derived "toxicity values" be consistent with or based upon federal (i.e., EPA) methodology and data? If so, are there any circumstances under which deviations from the federal (i.e., EPA) methodology and data should be allowed?

Question 7 was modified by the TAG to read as follows:

A. *If the EPA has not developed one or more toxicity values for a chemical, should the MDEQ attempt to evaluate developing the missing values?*

B. *If so, are there any circumstances under which deviations from the federal (i.e., EPA) methodology and data should be allowed?*

Summary Answer: Part A–Yes; the MDEQ should be allowed to develop and/or use toxicity values that were not derived by the EPA.

Part B–Yes; the MDEQ should be allowed to deviate from federal data when EPA data do not represent best available science. There are circumstances where EPA toxicity values are available, but not used to calculate generic criteria. Part 201 requires toxicity values be based on the best available science. The EPA, in general, has the resources to develop updated guidance, recommend methodologies, and derive toxicity values using those methodologies and the most current data. However, this is not the case for all toxicity values. Some recommended toxicity values are outdated and the EPA does not always speak with one voice. For example, the EPA Office of Drinking Water developed a Maximum Contaminant Level (MCL) many years ago that is not based on the most current science and is not consistent with newly revised values recommended in the EPA's Integrated Risk Information System (IRIS) database.

The TAG recommends tiered reference sources with the understanding that values will be reviewed to determine if it is reasonable to assume the values represent the best available science. For example, IRIS

is identified as the preferred source, with the condition that if the value in question is either outdated or there is information indicating, that it should be modified. The recommended approach is summarized in Appendix B.

Recommendation 10: The MDEQ should first determine whether a chemical is considered carcinogenic to humans by the EPA and International Agency for Research on Cancer (IARC). If it is to be regulated as a carcinogen, then potential route-specific differences in carcinogenicity should be considered and evaluated. If it is noncarcinogenic, then only the reference dose (RfD) and reference concentration (RfC) candidate values would be assembled to select an RfD and an RfC.

Recommendation 11: The criteria should be footnoted to denote whether the carcinogenic or non-carcinogenic algorithms are used to calculate the final criteria for a chemical.

Recommendation 12: Deviation from EPA methodology should be allowed where there is good information to suggest that the EPA's methodology or data are not consistent with current best science. Where these modifications are made by the MDEQ, there should be an opportunity for public input and comment, as described in Appendix C.

Discussion

The group had three different interpretations of what is being asked in the first part of Question 7. Some participants thought it referred only to MDEQ-derived values and not broader data sources. Other participants said they thought this was about establishing guidelines when Michigan's standards are stricter than EPA standards, with a goal of generally *not* having stricter standards than the EPA. Others thought it was asking about addressing missing endpoint values in the federal standards.

In response, a MDEQ representative provided context that this question's origins were in using cumulative risk with combined exposure pathways versus specific pathway screenings. This has been a controversial issue in the past, but because of the limited time frame for this current stakeholder process, the CSA does not want the TAG to address this entire issue, including the algorithms. Instead, it preferred that the TAG focus on a limited portion of the issue, and address whether the MDEQ should be consistent with federal methodology or whether the MDEQ should adopt its own methodology.

The group modified the question, as indicated above.

Question 8

Should an independent evaluation (by the MDEQ) of the chemical-specific data be conducted even if a value is published in the primary database of the hierarchy?

Summary Answer: Yes. The TAG agreed such independent evaluations are appropriate and are proposed to the MDEQ within the decision frameworks. Each chemical can be subject to an independent evaluation if required in order to be consistent with the best available science. For example, if a toxicity value is available in IRIS, but that value is no longer consistent with the current best available science, either the MDEQ or other interested party can bring forward data to be considered in revising or deriving a more appropriate value. The group recommends that the words "by the MDEQ" be added to this question so that it reads as it does above. This clarifies that the independent evaluation is the MDEQ's independent evaluation, which is met by going through the decision framework.

Question 9

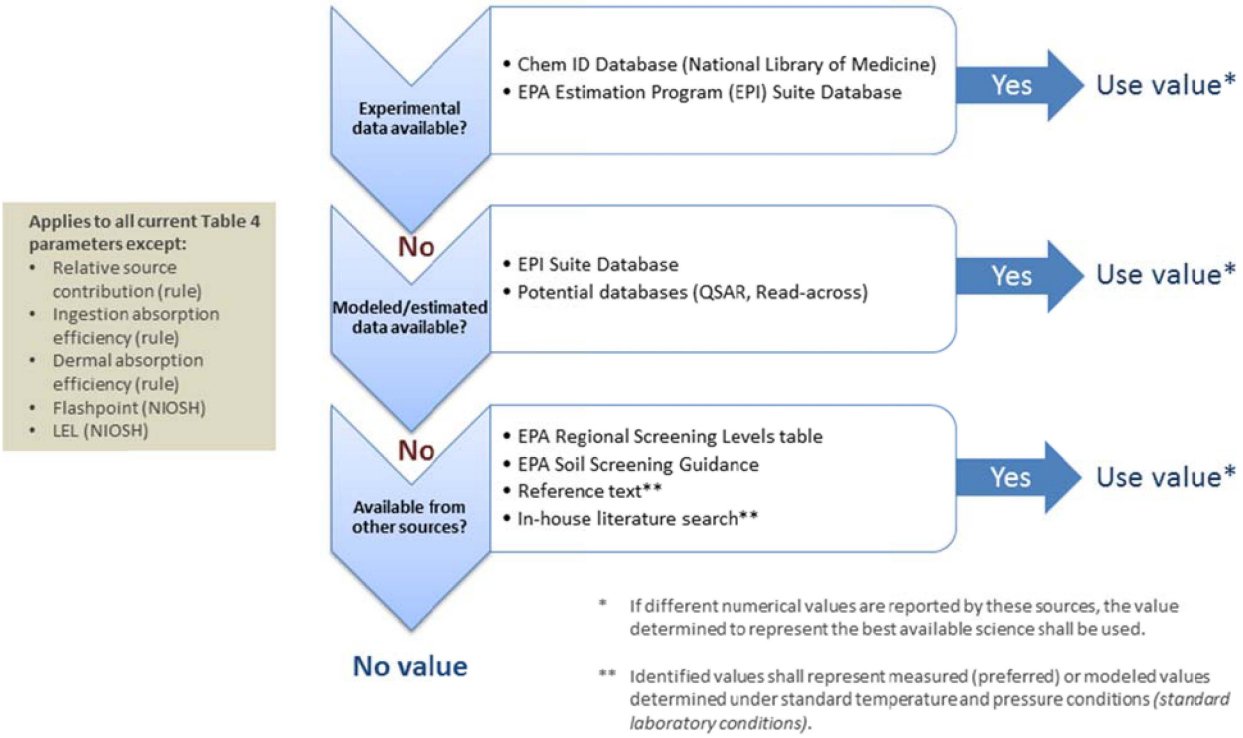
For chemical–physical parameters, should experimentally-derived values take precedence over theoretically-derived estimates?

Summary Answer: Generally, the TAG agrees that experimentally-derived values means experimental data that is the result of scientific experiments conducted in a controlled laboratory environment, typically at standard temperature and pressure; therefore, experimentally-derived values should take precedence over model theoretically-derived values whenever possible. The proposed decision frameworks establish which estimates take precedence when experimental data are unavailable (See discussion under Questions 1 and 5 and Appendices A and B). However, as discussed above, there was disagreement on how to select measured values from multiple valid measured values for physical-chemical parameters when these values differ significantly. This disagreement ultimately concluded in two different perspectives on how and where SSG should be used in a decision framework.

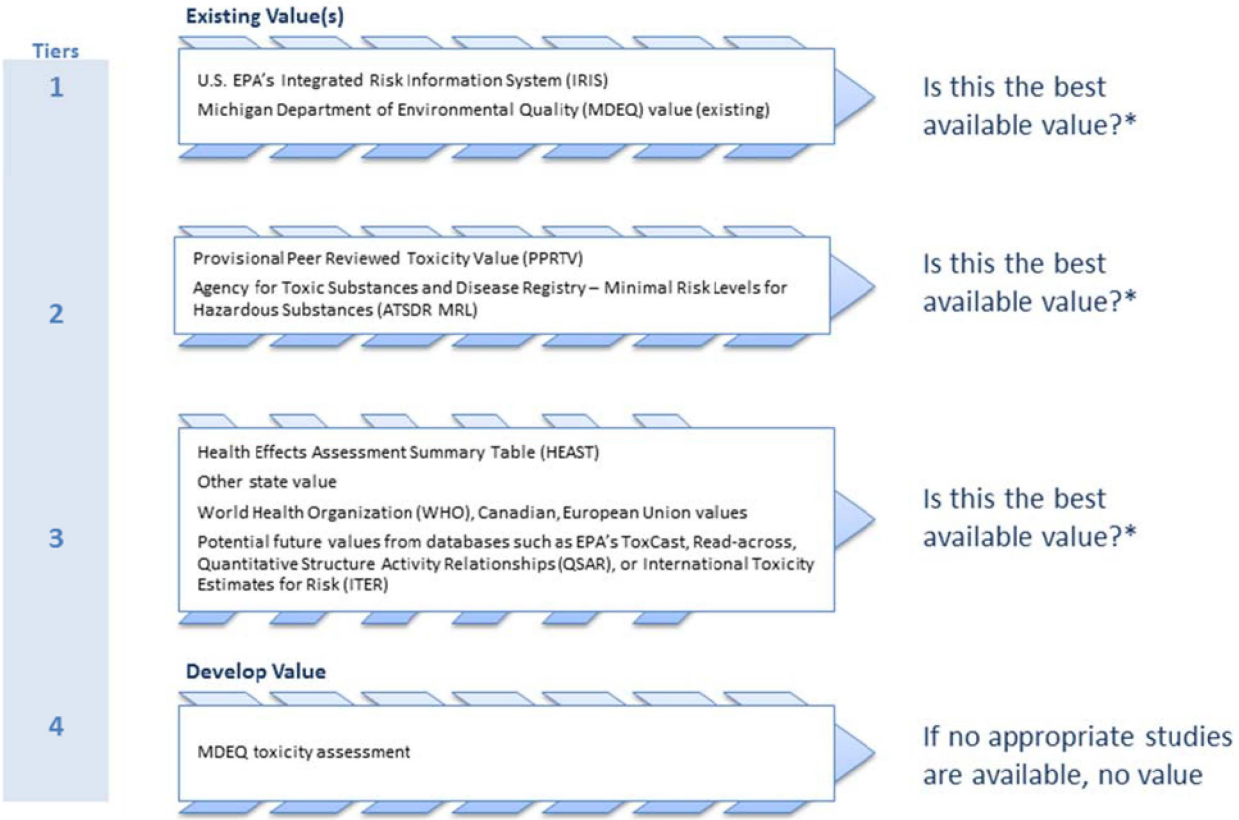
Appendices

- Appendix A: *Chemical–physical Value Decision Framework*
- Appendix B: *Toxicity Value Decision Framework*
- Appendix C: *Four-year Update Cycle*
- Appendix D: *Chemical Update Worksheet*
- Appendix E: *Soil Screening Guidance Background and Rationale for Differing Views*

Appendix A:
Chemical–physical Value Decision Framework



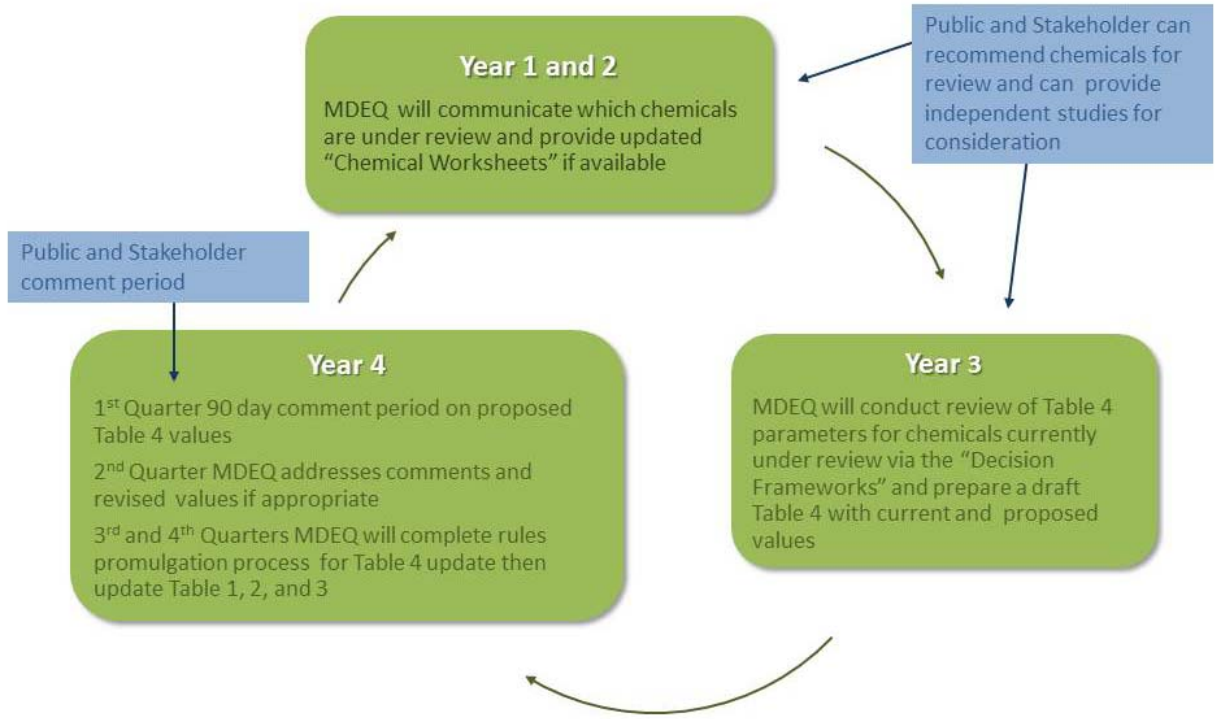
Appendix B:
Toxicity Value Decision Framework



* Values may have to be assessed for best available science (see TAG Recommendation 8)

Appendix C:
Four-year Update Cycle

MDEQ Four-year Update Cycle for Table No. 4



A proposal to update the toxicity and chemical-physical data presented in Table 4 (Toxicological and Chemical-Physical Data for Part 201 Generic Cleanup Criteria and Screening Levels) once every four years emerged from the TAG; it would allow for an open submission period (e.g., 3 years) and a petition process for chemicals to be considered for update in years 1, 2, and 3. In year 3, the MDEQ would identify which chemicals would be updated, based upon available information; in year 4, the department would allow a comment period and then move through the legislative rule process. It was noted that the MDEQ has internally discussed annually posting candidates (e.g., 5 to 10 chemicals a year that need to be re-evaluated). The candidate chemicals would come from an open submission period, a petition process for chemicals to be considered, and updated toxicity values that come through IRIS or other significant sources.

The TAG supported the proposal and emphasized the goal should be to ensure the regulated community, Michigan citizens, and the MDEQ are utilizing cleanup criteria that represent best practices, reasonable and realistic conditions, and sound science. In order for this update process to work, the language in the criteria rules would need to be revised to require a mandatory four-year update to Table 4 that, by reference, would cause Table 1 (Groundwater: Residential and Nonresidential Part 201 Generic Cleanup Criteria and Screening Levels), Table 2 (Soil: Residential; Part 201 Generic Cleanup Criteria and Screening Levels), and Table 3 (Nonresidential Part 201 Generic Cleanup Criteria and Screening Levels) to be updated, as well. The intention of the update every four years is to provide current toxicological and chemical-physical parameters. This approach is intended to be a balance between the MDEQ's expectation to update Table 4 in real-time (as the data are made available) and the regulated community's desire to have predictable cleanup criteria. The proposal offers an approach for the MDEQ to

communicate what chemicals it will evaluate within a predictable time frame. TAG members noted that while the process indicates that the MDEQ would provide notice every six months, the time period could be different (e.g., 12 months) and would be determined by MDEQ resources.

The Update Process

The proposed update process would occur over the course of four years and would be designed to improve transparency and communication of the chemicals the MDEQ would evaluate during a given cycle.

In year 1, the MDEQ would inform stakeholders that the update process is initiated, share a list of chemicals proposed for update, and provide stakeholders an opportunity to provide input. The MDEQ would solicit input from stakeholders on additional chemicals to review and relevant studies related to those chemicals.

In years 2 and 3, the MDEQ would review the chemical–physical and toxicity values for the proposed subset of the approximately 300 chemicals to evaluate the updated values or data submitted on the chemical.

In year 4, during the first quarter, proposed revisions to the values would be released for comment. In the second quarter, the proposed revisions and comments would be reviewed with stakeholders. In the third and fourth quarters, the revisions would go through the legislative process to complete the update of the criteria.

The TAG discussed if there were other administrative or legislative cycles that should be considered to determine when the four-year update process should begin. Members also discussed developing a mechanism for values to be re-evaluated on an emergency basis. Members agreed that a mechanism would be important and that consideration should be given to how "emergency" is defined. Members suggested that an emergency evaluation could be left to the joint discretion of the directors of the Departments of Community Health and Environmental Quality, when there is an immediate threat to public health.

TAG members discussed instances where ambiguity exists in some definitions (e.g., the definition of *substantial*) and suggested that the legal TAG should concur with language regarding an emergency update to criteria. Members noted that Michigan's Public Health Code may provide examples of language for similar provisions. The group also discussed whether or not a magnitude of change in values should be included in the emergency provision, and whether the language should provide examples of when an emergency action should be taken to help clarify what "emergency" means.

The TAG discussed when the four-year cycle should begin for revisions to the criteria that the MDEQ has had under development since 2009. The TAG noted that the department has a legislative mandate to update the criteria. Members agreed that the TAG should acknowledge that the review process for current updates may present a challenge, but that once new criteria are in place, the proposed four-year update process should be effective.

The group discussed two potential approaches to adopt the updated criteria the MDEQ has been working on since 2009. Under the first approach, proposed updates could begin at year 3 of the four-year cycle. However, the TAG noted that this approach may not meet the mandated time frame to update the criteria.

Under the second approach, the updated criteria could be adopted in a shorter time frame, with a grandfather clause, and a new four-year review cycle would begin at that time. The TAG discussed how sites existing within an approved remedial or corrective action plan (or similar plan) would be addressed when updated criteria are adopted. The goal is to establish a bright line for existing sites with agreed-upon

criteria where cleanup activities have occurred, as opposed to *new* sites as criteria are updated into the future. The group also noted that additional consideration would need to be given to smaller *due care* sites using such an approach. The TAG indicated, however, that the review period under this approach may provide a relatively brief time to review and comment on proposed updates.

The TAG identified the following matters that should be considered further by TAG 4 (Legal):

- If the rule establishes a mechanism to update criteria, do updates need to go through the full rule-making process?
- Consider and develop language regarding a provision that would allow for emergency updates to criteria in special circumstances with a clear public health urgency that would include both actual exposure and short-term potential for harm
- The MDEQ should formalize a process to include a provision that would allow a responsible party to apply for site-specific criteria within a specified period of time that would grandfather a site under the former criteria and approved cleanup plan.

The TAG acknowledged that the process used to implement the next update to the criteria may create challenges, but that once new criteria are in place, the proposed four-year update process should be effective. The challenge in updating the process will be in providing adequate time to review and comment on the updates, while adhering to the legislatively mandated time frame to adopt updated criteria. Those in charge of the initial update process should be mindful of the full extent to which criteria can be updated, given MDEQ resources available and the fact that the values have not been updated since 2002.

Documentation

- The MDEQ should provide references for all values listed in Table 4 (e.g., IRIS, MDEQ-derived, ATSDR, ChemIDplus, or other specified references) (Recommendation 2).
- The MDEQ should notify stakeholders and post on its website a list of proposed chemicals and values for update in Table 4 (Recommendation 6).

Communication

- The MDEQ should provide notice via website or e-mail listserv every six months of potential new updates to Table 4. This update will list the chemical(s) affected, and provide a link to the current Chemical Worksheet(s). These updates will not take effect until year four of the update cycle (Recommendation 6).
- Annually, the MDEQ should solicit input from the regulated community and stakeholder groups for chemical(s) the MDEQ should review in a given year, as well as solicit and respond to comments on updates that the MDEQ has proposed that are not yet put into place. Based on current MDEQ staff levels, the MDEQ would likely perform a detailed review of only five to 10 chemicals per year. The MDEQ would provide a response to input received (Recommendation 3).
- The MDEQ should document the basis for selection of proposed updated values, including what values were available and why the identified values were selected, including, but not limited to, rationales for selecting a different toxicity value when an IRIS or Provisional Peer Reviewed Toxicity Value (PPRTV) is available (Recommendation 6).
- Final revised Table 4 values will be documented in chemical update worksheets, which will summarize the selection process for modified values (Recommendation 6).
- Recognizing that the focus of this TAG is generic criteria, when site-specific criteria are being developed, members recommended that the MDEQ provide a form for use in the same format as the

chemical update worksheet, to be filled out by the user. If site-specific criteria are approved, the form will be shared on the MDEQ website. (TAG members discussed the intent of this recommendation, which is to improve transparency by providing information about approved site-specific criteria so others that may have similar site conditions can be aware of the approval of the site-specific criteria.)

Appendix D:
Chemical Update Worksheet

CHEMICAL UPDATE WORKSHEET

Chemical Name:	
CAS #:	
Update Date:	

(A) CHEMICAL-PHYSICAL PROPERTIES

	Part 201 Value	Updated Value	Source/ Reference/Date	Comments/Notes/Issues
Molecular Weight (g/mol)				
Physical State at ambient temp				
Melting Point (˚C)				
Boiling Point (˚C)				
Solubility (ug/L)				
HLC (atm-m³/mol at 25˚C)				
Log Kow (log P; octanol-water)				
Koc (organic carbon; L/Kg)				
Diffusivity in Air (Di; cm^2/s)				
Diffusivity in Water (Dw; cm^2/s)				
Soil Water Partition Coefficient (Kd; inorganics)				
Flash Point (˚F)				
Lower Explosivity Level (LEL; unitless)				

(B) TOXICITY VALUES/BENCHMARKS

	Part 201 Value	Updated Value	Source/Reference/Date
State Drinking Water Standard (ug/L)			
Secondary Maximum Contaminant Level (ug/L)			
Aesthetic Drinking Water Criterion (ug/L)			
Reference Dose (RfD; mg/kg/day)			
RfD Details			
Oral Cancer Slope Factor (CSF; $(mg/kg\text{-}day)^{-1}$)			
CSF details			
Initial Threshold Screening Level (ITSL; ug/m^3)			
ITSL averaging time			
ITSL details			
Inhalation Unit Risk Factor (IURF; $(ug/m^3)^{-1}$)			
IURF details			
Reproductive Effector? (Y/N)			
Reproductive Toxicity Details			
Developmental Effector? (Y/N)			
Developmental Toxicity Details			
Aesthetic Value or Comments			
Phytotoxicity Value			
Other			

(C) RULE 57 WATER QUALITY VALUES AND GSI CRITERIA

1. Surface Water Assessment Section Rule 57 website
2. Rule 57 table

Current GSI value (µg/L)	
Updated GSI value (µg/L)	
Rule 57 Drinking Water Value (µg/L)	

	Rule 57 Value (µg/L)	**Verification Date**
Human Non-cancer Values- Drinking water source (HNV-drink)		
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)		
Wildlife Value (WV)		
Human Cancer Values for Drinking Water Source (HCV-drink)		
Human Cancer values for non-drinking water source (HCV-Non-drink)		
Final Chronic Value (FCV)		
Aquatic maximum value (AMV)		
Final Acute Value (FAV)		

(D) ANALYTICAL INFORMATION

Target Detection Limit – Soil (µg/kg)	
Target Detection Limit – Water (µg/L)	

Appendix E:
Soil Screening Guidance Background and Rationale for Differing Views

Background

Two differing views emerged among TAG members with respect to using the Soil Screening Guidance (SSG) for the selection of physical–chemical parameters and whether it was appropriately positioned in the Decision Framework (Appendix A). The two views held by TAG members differed and point out an apparent inconsistency between the recommendations of one TAG member to use the SSG and SSG's methodology to select values for physical/chemical parameters and text in the Supplemental Soil Screening Guidance (Supplemental SSG) that states the toxicity values and physical/chemical parameters should be checked for any potential updates before use.

Differing Views

Rationale to support the TAG's prevailing view:

In 1996, the EPA issued the Soil Screening Guidance document (original SSG) which presented, in part, chemical-physical data relevant to the most commonly identified chemicals at National Priorities List (NPL) sites. These data were intended to be used in the development of health protective soil screening levels at NPL sites. In 2002, the EPA issued the Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites document (supplemental SSG), a companion document to the original SSG, which also contained chemical-physical data intended for use in developing health protective soil screening levels.

The methods, models, and data presented in the original (1996) and supplemental (2002) SSG documents were not intended to be used in perpetuity as originally published. The supplemental SSG document itself recommends that users check the most recent versions of the appropriate sources for updated regulatory/health benchmarks (e.g., toxicity values) and chemical-physical properties to confirm that the most current values are being used. Per Appendix C of the supplemental SSG document,

> "All of the sources of the values listed in Exhibits C-1 through C-5 are regularly updated by EPA. In addition, the information in Exhibits C-6 and C-7 was obtained from RAGS, Part E. Therefore, prior to calculating SSLs for a site, regulatory/health benchmarks and chemical properties should be checked against the most recent versions of the appropriate sources to ensure that they are up to date."

Appendix C then directs the reader to check online sources, including the EPA Integrated Risk Information System (IRIS), the National Primary Drinking Water Regulations, Superfund Chemical Data Matrix Report (SCDM), CHEMDAT8, and WATER8; all resources used to populate the toxicity and chemical-physical values in the document.

Since issuance of the 2002 supplemental SSG document, the EPA has continued to advance the science that it uses to develop its health protective soil and water screening levels. This is supported by the following discussions.

- The EPA has continued to conduct health assessments of new and existing chemical substances, which are published in the online IRIS database.

- The EPA revised the National Primary Drinking Waters Standard for inorganic arsenic from 50 parts per billion (ppb) to 10 ppb on January 23, 2006.
- The most current version of SCDM was published online in June 2014. While "Part 2 – Data Selection Methodology" of SCDM does reference the supplemental SSG document for some chemical-physical parameters, it is typically identified as a lower preference data resource. Syracuse Research Corporation's PHYSPROP database (embedded in the EPA's EPI Suite database) and the EPA's EPI Suite database itself are consistently given higher preference as chemical-physical data resources by SCDM. This order of preference and recommendations for use (e.g., measured values preferred over estimated values) are consistent with the chemical-physical decision framework presented in the TAG1 Final Report.
- Per the EPA's WATER9 (version 2.0) model website, the WATER8 and CHEMDAT8 models referenced in the 2002 supplemental SSG have been superseded by WATER9. It is stated on the WATER9 website that "WATER9 is a significant upgrade of features previously obtained in the computer programs WATER8, Chem9, and Chemdat8."
- The May 2014 EPA Regional Screening Level (RSL) Chemical-specific Parameters Supporting Table primarily references the EPA EPI Suite database and WATER9 model as the sources of chemical-physical data used in calculating the RSLs. However, the RSL User's Guide references the soil-water partition coefficient for metals (i.e., Kd) parameter to the supplemental SSG. This is consistent with the approach presented in the TAG1 Final Report chemical-physical decision framework.
- Comparison of measured values in the supplemental SSG to modeled or estimated values in EPI Suite is misleading as measured values can be found in both the SSG and EPI Suite. It should also be noted that the same database, maintained by the Syracuse Research Corporation, is the source for both the supplemental SSG and EPI Suite. Additionally, primary literature citations are available in EPI Suite, but not listed in the supplemental SSG. Use of EPI Suite would allow greater transparency for stakeholders examining the origin of specific chemical parameters.

<u>Rationale to support a TAG member alternative view of the SSG for selection of physical/chemical values</u>

To date, the Part 201 program generally has been using the most scientifically sound, robust, and reputable sources for physical/chemical parameters because it uses the recommended values from EPA's SSG and uses values from the SSG-recommended sources for chemicals that were not specifically listed in the SSG. Physical chemistry values are generally static and therefore not subject to intensive ongoing research in the same way that toxicity values are and as such, the values that are in place now in the generic criteria are up-to-date and correct.

MDEQ's rationale for adopting this EPA guidance was documented in Attachment B of Op Memo No. 18 (August 21, 1998). Although the SSG recommendations were based on a robust and technically sound evaluation, deviations from the recommendations may be justifiable for specific chemicals or parameters on the basis of chemical- or parameter-specific considerations (e.g., an emerging contaminant). MDEQ should have a process for evaluating requests for such deviations, as well as for establishing parameter values when a value is not given in the SSG, cannot be derived by using the methods recommended in the SSG (e.g., deriving Koc values from Kow values), and is not available in the SSG-recommended sources. This process can follow the Generic Criteria Physical-Chemical Value Decision Framework and would involve the evaluation of scientific information specific to the parameter in question. The rationale for establishing a value on the basis of this information should be transparent and well documented.

Although the SSG is from 1996 and was updated in 2002, its recommendations for the selection of physical–chemical parameters are still more robust and scientifically sound than any other subsequent EPA guidance because the recommendations were based on an extensive evaluation of many sources of physical–chemical values, addressed the difficult issue of selecting a value from multiple, valid measurements, were subject to extensive public comments, and are well documented (see SSG: Technical Background Document, Part 5: Chemical-Specific Parameters). As such, the SSG values and the recommended hierarchy of sources should continue to be first choice in deriving Part 201 generic criteria, although deviations from the SSG recommendations on a parameter-by-parameter basis may be valid, and certain parameters specific to the dermal route (ABS_{derm} and FA) should be taken from RAGS Part E (Dermal Guidance, 2004) which was also based on a rigorous evaluation (i.e., peer reviewed) and subject to extensive public notice and comments.

The following example (using K_{oc} for benzene) illustrates why the SSG remains the most robust source for selecting default values for physical/chemical parameters, as compared to alternate sources such as EPI Suite or ChemIDPlus:

- EPA recognized that it must address the issue of selecting a single value from among the multiple valid measured values found in the literature (including those in Syracuse Research Corporation databases), which may span a wide range of values for many chemicals.
- EPA recognized that K_{oc} can be difficult to measure, and as a result, measured values are available for a limited list of chemicals, and the measurements for some chemicals are variable (for benzene the range EPA evaluated after removing outliers was from 31 to 100 L/kg).
- EPA recognized that K_{oc} is strongly related to K_{ow}, and measured K_{ow} values are more readily available and can be used to estimate K_{oc} values (Section 5.3.1 of the SSG cites the work of Lyman and DiToro as the basis for using a linear regression of measured values for chemicals of concern at Superfund sites).
- EPA presented two regression equations of log K_{ow} to log K_{oc} for calculating K_{oc} based on measured K_{ow} values that showed good correlation for the chemicals in the different chemical classes associated with each regression equation; and
- These equations were used in SSG to provide a consistent means of addressing variability among the measured K_{oc} values for a given chemical and filling gaps in the K_{oc} dataset for chemicals that lack measured K_{oc} values but have measured K_{ow} values.

The above examples demonstrate that the values contained within the SSG were derived through relevant and accepted methods, are credible, and are based on experimental data. Further, in total the SSG is a comprehensive source as it provides physical-chemical values for numerous chemicals and a procedure for selection of values for chemicals not included in the SSG.

As an alternative to the SSG, the TAG considered using the measured value(s) included in EPI Suite. However, attributing the values contained within EPI Suite to EPI Suite would be incorrect and even misleading, for the following reasons (continuing with the benzene K_{oc} example):

- The K_{oc} of 56.2 L/kg included in EPI Suite is not generated by the prediction algorithms in EPI Suite, which per the software documentation is the sole purpose of the EPI Suite software, and the program provides no documentation on how or why this value was selected.
- As indicated in the EPI Suite documentation, the K_{oc} of 56.2 L/kg is actually a 1991 measured value from the Syracuse Research Corporation (SRC), presumably included in EPI Suite as a point of

reference for judging the values predicted by EPI Suite, and is only one of at least 13 measured K_{oc} values for benzene that EPA included in the development of its recommendations in the SSG.

The TAG further considered using online databases such as ChemIDplus for identifying default values for certain parameters. However, ChemIDplus has limitations that are similar to those associated with attributing measured values to EPI Suite. Specifically, ChemIDplus appears to prefer values from SRC (while providing no basis for selection of these values), which is only one of the many sources EPA included in its evaluation in the SSG, and as such, is less robust and less scientifically sound. Continuing with benzene as an example, the values for various parameters from SRC are cited to studies published between 1979 and 1995 that EPA included in the development of its recommendations in the SSG.

The TAG also considered using prediction methods from EPI Suite. However, the measured and prediction results from EPI Suite are less robust and less scientifically sound than those from the SSG, for the following reasons (continuing with the benzene K_{oc} example):

- EPI Suite predicts two K_{oc} values for benzene (145.8 and 70.51 L/kg) and provides no guidance or recommendation on which value to use.
- The predicted value of 145.8 L/kg is outside the measured range for benzene, as documented in the SSG.
- The other predicted value is apparently estimated using a correlation to K_{ow}, which is similar to the correlation recommended in the SSG, but lacks information on its basis and source (e.g., what chemicals were used in the regression, and how good was the fit).

<u>Response to comments from TAG members not supporting the continued use of SSG as the primary source of physical-chemical values</u>

The main point of the comments from the TAG seems to be pointing out an *apparent* inconsistency between the recommendations to use the SSG and SSG's methodology to select values for physical-chemical parameters and text in the Supplemental SSG that could be interpreted to read that EPA believes that the values for physical/chemical parameters are routinely modified.

The statement from the Supplemental SSG that reads, "All of the sources of the values listed in Exhibits C-1 through C-5 are regularly updated by EPA." does not accurately characterize EPA's actual practice as it relates to physical-chemical parameters. The values in Exhibit C-5 of the Supplemental SSG (toxicity values) are routinely updated as new toxicity studies emerge. But the updating of toxicity values (which is the subject of the first two bullets in Appendix F) is not relevant to the discussion of physical-chemical parameters. The physical-chemical values in Exhibits C-1 through C-4, specifically Koc, solubility, henry's law constant, melting point, Kd, and diffusivities are generally considered static and little or no new research is available for these values. The values in Exhibit C-1 to C-4 of the Supplemental SSG demonstrate this. A comparison of the values in Exhibit C-1 to C4 with those in the 1996 SSG shows that the two sets of values are the same; none of the values for the parameters in Exhibit C-1 to C4 changed between the 1996 SSG and the 2002 Supplemental SSG. Therefore, the EPA statement quoted above applies to the toxicity values in Exhibit C-5 but does not apply to the physical-chemical parameters.

The inaccuracy of the above quoted statement relative to physical-chemical parameters is further demonstrated by investigating the source of the values provided in both EPI Suite and ChemIDPlus. Using the example of benzene from the original proposed text shows that the most recent cited study from either of these sources is from 1995, which predates both the SSG and the Supplemental SSG.

In principle, EPI Suite is a reasonable source where acceptable measured values are not available. However, the text provided above describes the merits of using the SSG approach (with benzene as an example) to illustrate some of the many ways that EPA identified and used acceptable measured values in making its recommendations, which remain valid. EPA's sources of acceptable values included SRCs PHYSPROP database as well as 12 other sources of measured values of Koc for benzene. EPA then used the proven relationship between Kow and Koc to develop a correlation that relies on measured values of Kow to calculate Koc values that honor this physical relationship. Therefore, the SSG approach for deriving Koc relies on literature to derive values based on measured Kow.

While the new methodology document from SCDM does identify that it uses a new approach for selecting Koc values, we were unable to find within the SCDM documentation any rationale for why it now believes the approach for calculating Koc should be modified to prefer the MCI estimation methodology (which existed at the time the SSG was written) over the log Kow method used in the SSG.