

Development of an Herbicide Properties Tool to Communicate Physiochemical
Properties of Pesticide Active Ingredients

by
Jamie Merritt

A THESIS

submitted to

Oregon State University

University Honors College

in partial fulfillment of
the requirements for the
degree of

Honors Baccalaureate of Science in Environmental Sciences
(Honors Scholar)

Honors Baccalaureate of Arts in International Studies
(Honors Scholar)

Presented February 25, 2016
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AN ABSTRACT OF THE THESIS OF

Jamie Merritt for the degree of Honors Baccalaureate of Science in Environmental Sciences and Honors Baccalaureate of Arts in International Studies presented on February 25, 2016. Title: Development of an Herbicide Properties Tool to Communicate Physiochemical Properties of Pesticide Active Ingredients .

Abstract approved: _____

Dave Stone

The National Pesticide Information Center (NPIC) is a cooperative agreement between Oregon State University and the U.S. Environmental Protection Agency that offers science-based information about pesticides and related topics to the general public, medical personnel, applicators, researchers, and regulators. The Herbicide Properties Tool project is the creation of an updated version of a popular database provided by NPIC. Using mainly primary source EPA documents, I compiled physiochemical data for 228 herbicide active ingredients that will feed into an easily understandable database. The purpose of the database is not only to update the previous version with new active ingredients but also to provide more information about the data for the general public to understand without a science background. For each active ingredient, the database will display data for water solubility, vapor pressure, soil half-life, sorption coefficient, and hydrolysis half-life. A groundwater ubiquity score and movement rating were calculated for each active ingredient to allow comparisons between two or more herbicide products.

Key Words: herbicides, pesticides, NPIC, database, tool, physiochemical properties, groundwater ubiquity score, groundwater movement

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I understand that my project will become part of the permanent collection of Oregon State University, University Honors College. My signature below authorizes release of my project to any reader upon request.

Jamie Merritt, Author

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Development of an Herbicide Properties Tool to Communicate Physiochemical Properties of Pesticide Active Ingredients

INTRODUCTION

Pest control applicators, agricultural workers, and other occupational pesticide users must understand the effects of their pesticides before use. Others who use pesticides may want to compare two or more pesticides in order to choose the option that poses the least risk to groundwater. Information about different pesticides is difficult to find from a product label or website. However, the U.S. Environmental Protection Agency (EPA) requires each pesticide product that is distributed, used, or sold in the U.S. to be registered through a scientific and legal procedure under the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA)¹. This act passed in 1996 requires all applicants to show that using the pesticide “will not generally cause unreasonable adverse effects on the environment.” FIFRA defines the term “unreasonable adverse effects on the environment” to mean: “(1) any unreasonable risk to man or the environment, taking into account the economic, social, and environmental costs and benefits of the use of any pesticide, or (2) a human dietary risk from residues that result from a use of a pesticide in or on any food inconsistent with the standard under section 408 of the Federal Food, Drug, and Cosmetic Act.” A company must submit an application when registering a new pesticide active ingredient, a new product, or adding a new use to an existing product. The evaluation process by the Environmental Fate and Effects Division (EFED) of the EPA looks for the following risks:²

- Aggregate risks
- Occupational risks
- Potential for ground water contamination
- Risks to endangered and threatened species

- Potential for endocrine-disruption

After evaluation, the EPA publishes a Registration Eligibility Decision (RED) for anyone to access through a federal database.³ These documents address the need for pesticide information but are difficult to find.

The National Pesticide Information Center (NPIC)⁴ is a cooperative agreement between Oregon State University and the U.S. Environmental Protection Agency that offers science-based information about pesticides and related topics to the general public, medical personnel, applicators, researchers, and regulators. Since 1999, NPIC has hosted a Pesticide Property Database (PPD)⁵ on their website to address the need of active ingredient information. This database includes a list of active ingredients with their corresponding soil half-life, water solubility, sorption coefficient, and movement rating or groundwater ubiquity score (GUS). The GUS is a derived value that allows users to compare the groundwater movement of active ingredients.⁶ This database has been a popular feature on the NPIC website and has been viewed over 33,000 times in eight years on the site. Professional applicators and educators have requested an update that would add new active ingredients. In addition, non-professional users are in need of a more convenient and understandable resource for pesticide information.

In order to meet these needs, a new database will be created and accessible through the NPIC website. The NPIC Herbicide Properties Tool is designed to provide users with useful data in order to analyze the potential groundwater and surface water movement of pesticide active ingredients. The goal of this project is to create a unique resource that is visually appealing and easily accessible and understandable. It will be flexibly designed for desktop and mobile devices, and thoroughly referenced. Similar databases are available and meet the need for technical information.⁷ However, these similar databases are generally more difficult to navigate and understand without a science background. The NPIC

Herbicide Properties Tool is interactive with links to definitions and explanations that target the 8th grade reading level. A professional resource will now be accessible to the general public as well.

In an effort to remain as reliable as possible, primary source data from EPA registration documents is predominantly used in the database. During this initial phase of development, only herbicides are under observation, excluding biopesticides. Herbicides were selected for priority evaluation in response to requests from pesticide users and the highest rate(s) of detection in surface water, compared to other pesticide types. In the future, NPIC hopes to expand the project to include other types of pesticides.

METHODS

Choosing Active Ingredients

The active ingredients (AIs) included in our database were those found in at least one pesticide product labeled “herbicide” in the Pesticide Product Information System (PPIS)⁸. This generated a 790-item list. If there were multiple items with the same PC Code, they were considered synonymous and the most pronounceable AI name was selected. In order to remove cancelled/banned AIs, NPIC searched for each AI using a database developed by NPIC called “NPIC Pesticide Research Online” or “NPRO.”⁹ We excluded AIs with no actively registered herbicide products. AIs represented as disinfectants or used to kill slime were excluded. Examples include AIs in paint used on boat bottoms to control marine organisms. AIs used to kill moss and/or roots were included. AIs that had many different versions, such as 2,4-D and dicamba, were included with all of the variations with actively registered products. For example, we searched for chemical properties for eight unique salts or esters of 2,4-D. The final list includes 229 AIs, 49 of which are ester or salt variations of the parent AI.

Choosing Properties

During initial collection, we attempted to find data for the following properties: aerobic soil metabolism half-life, hydrolysis half-life, log K_{ow} , anaerobic aquatic metabolism half-life, K_{oc} , water solubility, foliar half-life, pK_a , and vapor pressure.

After searching for primary data sources according to the protocol described in the next section, the following properties were kept in the table because data gaps were acceptably low and they were considered vital in order to convey fate and transport information to the audience: aerobic soil metabolism half-life, vapor pressure, K_{oc} , water

solubility, and hydrolysis half-life. The additional four properties were removed from the table because little data were found.

In order to provide users with a means to compare potential movement and ground water contamination, the GUS is displayed for each AI. Each chemical's potential is categorized low to high. The GUS is calculated for each AI in the database, following the methods and using the equation outlined below:⁶

$$\text{GUS} = \log (\text{soil half life}) \times (4 - \log K_{oc})$$

The GUS is a conditional value and dependent on soil type and circumstance. Because of this, the soil half-life and K_{oc} values are recorded with different soil types. The three soil types found are sandy soils, silty/loam soils, and clay soils. Other factors that may affect the AI groundwater movement are temperature, moisture, organic matter content, pH, sunlight, and microbial activity.¹⁰

We wrote brief explanations about each property explaining why it is important in determining groundwater safety that is viewable when the user hovers over the property title. In addition, NPIC fact sheets for water solubility and soil half-life are linked to the property title in the database by clicking it. (Appendix A)

Collecting Data

NPIC chose to mainly utilize primary source data through the HPT, meaning sources that present data from original research and experiments are cited. If a primary source was not found initially then secondary sources were searched. For each AI, the process of collecting data began with searching for the ingredient in the NPIC Product Research Online Database (NPRO) to record the CAS Registry number. Next, we used the CAS Registry

Number to search for each AI in an EPA database called ChemSearch.¹¹ From this site, we found identification numbers that allowed us to locate data-rich EPA Dockets for each AI.³ The primary sources of data were EPA documents including Registration Eligibility Decisions (REDs) and Environmental Fate and Effects Division Risk Assessments (EFED RAs). These were considered primary because these data are experimentally derived by pesticide registrants and provided directly to EPA. Within the EFED RAs, most of the physical property data could be found in the Environmental Fate and Transport section. The EFED was the most common source to find physical/chemical properties for an AI.

If the desired data was not found within EPA documents, then we searched an internal database of AI documents called InfoBase. The Info Base resources frequently included information re: toxicology studies, ecological risk assessments, and archived documents not readily available in the EPA docket(s).

If no data were found among EPA documents or NPIC's InfoBase, then SciFinder database was queried. Using the CAS number to search for an AI, only primary sources were used from this database. If a secondary source was found, the information was tracked back to the original source.

Finally, if unsuccessful with these online databases, data were obtained from the 10th edition of The Herbicide Handbook.¹² Although this is not a primary source, it is considered a reliable secondary source used only to fill gaps. Roughly eleven percent of the data in the spreadsheet was found in the Herbicide Handbook.

Limitations arose during data collection when a range of data was available. Because we could not perform calculations on ranges of data, the middle value in a range was selected to calculate the GUS. Another limitation arose when performing GUS calculations. In some cases, the K_{oc} value would be available for soil specific data while the aerobic soil metabolism half-life would only be available for unknown soil types or vice versa. In these

situations, the unknown soil type value was used with the soil specific value to calculate a soil specific GUS. Because of this, we have included text in the database stating, "The GUS value was calculated using the most soil-specific values available. If the soil type were unknown for the half-life and K_{oc} , the GUS value would appear with an "unknown soil type" heading. If one or both of the properties (half-life, K_{oc}) were published with known soil types, the GUS value would appear with a soil-specific heading".

Citing Data

With the exception of copyrighted material, data files were saved in Portable Digital Format (pdf) with destinations set to pertinent sections of each document. Each destination was later referenced using a unique URL and references were tracked for each chemical property recorded.

Designing the Database

Subject matter experts, graphic artists, and developers collaborated to create a two-tiered user interface. The first tier has two options: the default is a list of each AI and the second looks like a simple table in order to meet the expectations of loyal users of the OSU Pesticide Properties Database. The second tier appears after an AI is clicked. It includes qualitative descriptors for some values, and graphic animations for others. In addition, a reference link appears with each value. Images and animations were created using Adobe Illustrator©. Qualitative descriptors were assigned as described in Table 1.

RESULTS

Five properties were sufficiently available and critical for assessing potential pesticide movement, including aerobic soil metabolism (in days), soil organic carbon-water partitioning coefficient (in mL/g, also known as a soil sorption coefficient), hydrolysis half-life (in days), vapor pressure (in mm Hg), and water solubility (in mg/L @ 25° C).

According to EPA documents, the salt and ester forms of parent active ingredients degrade quickly to form the parent acid in most environmental conditions. Consequently, the salt and ester forms can be lumped to the parent acid and all reported physiochemical properties relate to every form of the ingredient. An example of an EPA explanation of the lumping of salts and ester is as follows: “The laboratory bridging data indicate that under most environmental conditions, 2,4-D esters and 2,4-D amine salts will degrade rapidly to form 2,4-D acid.”¹³ When a compound’s salts and esters were lumped with the parent ingredient, there were 180 AIs. When they were evaluated separately, there were 228 AIs.

Of the 180 herbicide ingredients, each of the four prioritized properties was found for 116 active ingredients. At least one datum point was not found for sixty-four active ingredients. Out of the 180 AIs, aerobic soil metabolism half-life data were not found for 17%, K_{oc} data were not found for 31%, vapor pressure data were not found for 7%, hydrolysis half-life data were not found for 34%, and water solubility data were not found for 6%. These percentages reflect the data not found from primary sources and the other resources used for data collection after a thorough search.

Because soil half-life and K_{oc} values are different under different conditions, we looked at three different soil types for these two properties including sandy, silty/loam, and clay soils. When the soil half-life or K_{oc} value was not specific to a soil type, the data were

categorized for unknown soil type. Soil specific data were found for 37% of the active ingredients.

The GUS was calculated for each soil type or unknown soil type with each AI. A GUS was calculated for 63% of the AIs. A GUS was not calculated if either the soil half-life or K_{oc} was not found for an AI. Based on the GUS value, we assigned each AI a movement score based on criteria in Table 2. The movement score allows users to compare the GUS of two or more AIs. It also eliminates a purely numerical representation of the groundwater movement and allows those without science knowledge to understand.

DISCUSSION

International Pesticide Policy

The United States has very different policy regarding pesticides in comparison to other nations. In the last fifty years, pesticide use in the U.S. has increased from 196 million pounds of active ingredient to 516 million pounds. This increase can be attributed to an increase in the total planted acreage of corn, wheat, and soybeans.¹⁴ With a growing use of pesticides, there has also been an increase in pushback from society towards the increased and potential for harm to human health and the environment. Since the 1960's, the U.S. has implemented numerous regulatory actions toward pesticide safety such as FIFRA, the Food Quality Protection Act of 1996¹⁵, the EPA registration process, and stricter labeling rules.¹⁶ Even with the new policies, the U.S. remains a top agricultural country and continues to use many types of pesticides. While toxicity is variable when it comes to pesticides, if the benefits outweigh the risks then the pesticide will most likely be used.

Canada follows similar standards as the U.S. It strictly regulates pesticides through the Pest Management Regulatory Agency (PMRA).¹⁷ PMRA registers all pesticides, reevaluates each AI currently on the market every fifteen years, and promotes sustainable pest management. The screening process for each AI is extremely detailed to ensure accurate and standardized submissions. However, unless there is substantial evidence of risk of an AI, the pesticide is registered for use, much like the U.S. policy.¹⁸

U.S. and Canada have been scrutinized for their national registration of some pesticides that have been banned or withdrawn in other nations due to health or environmental concerns.¹⁹ The European Union (EU) in particular bans many more pesticides than the U.S. or Canada. The number of banned or severely restricted AIs in the EU is 168 while it is 65 in the U.S.²⁰ In 2001, the European Commission implemented the

White Paper strategy for chemical use with the main objective to guarantee high level protection for human and environmental health. This initiative set up an approach to phase out all harmful substances and replace them with progressive, sustainable alternatives.²¹ In 2007, the new EU chemicals regulation was implemented to regulate, evaluate, authorize, and restrict chemicals (REACH) according to the White Paper strategy.²² In general, the EU is stricter with pesticide restriction than the U.S. and Canada.

In comparison to these developed countries, developing countries use more pesticides in order to reduce pest-induced food losses. Their policies tend to be less strict because food production is considered essential for economic development and general stability. As populations continue to rise in these countries and in general, I anticipate pesticide use to increase immensely in developing countries in the future.

Although each country has a different set of rules and regulations set towards pesticides and other chemicals, this Herbicide Properties Tool will be useful to anyone around the world looking for physiochemical data of active ingredients. Looking at NPIC user statistics from 2015, 16% of the people accessing the NPIC web pages during the year were from outside of the U.S. The top six nations, other than the U.S. that accessed this site since its launch eight years ago have been Canada, India, Great Britain, Australia, Mexico, and China. This database can be used by anyone worldwide. Due to the rising population in every country, agriculture will remain a very significant aspect of human culture, which means pesticides will remain an important topic as well.

Impact

A reliable and credible source of active ingredient properties that enable comparison between chemicals has been developed based on the work of this thesis. The

research was necessary because there previously was no resource that compiled data from primary source EPA documents at this level of detail. This tool adds convenience to the search for physiochemical data. In addition, non-professional pesticide users were in need of a resource that explains more about their products than just numbers lacking useful context. This database will include explanations of how each piece of data was collected, what the number means, and a visual representation of what the property indicates. For example, the water solubility column for each AI will display the value along with an image of how much of the chemical mixes with water and how much remains as a precipitate. By gathering all of the data into one database, the viewers will also be able to compare the different AIs if they wish to pick one with less of an environmental impact.

Apart from informing the user of physiochemical values of AIs, this resource may also serve to remind pesticide users that all chemicals can affect environment. This database may lend to that opinion and display that pesticides not only affect the target but the surrounding environment as well. Some scenarios that may benefit from learning about the physiochemical properties of pesticides are when a user get his or her drinking water from a well, when animals spend a lot of time outside near a pesticide spray, or when two agriculture sites are close to each other. If a pesticide is highly soluble in water or has a long soil half-life, it can more easily join the groundwater stream and collect in wells or other sources of water. Depending on the pesticide, long-term ingestion of chemicals in water, which may occur if a well becomes contaminated, can cause long-term health effects such as cancer or organ damage.²³ Similarly, if a pesticide is used near a home or yard, any animals that spend extended amounts of time outside could be effected. In this situation, if the pesticide active ingredient has a high vaporization, the chemical could remain in the surrounding air for longer than expected. Pesticides move easily through the air and water, causing problems when two or more agricultural sites are situated near each other. For

example, an organic farm may reject the use of pesticides while the neighboring farm sprays pesticides often. Understanding how that specific pesticide moves and how long it remains in the environment is beneficial for both parties in order to prevent the movement of the AI from one farm to the other.

I hope that users will begin to utilize integrated pest management (IPM) more often than before. This is a method of pest management that minimizes the use of pesticides and encourages sustainable pest management strategies.²⁴ Of course pesticides are necessary in many situation, which is why this database will be useful; however, if they can be avoided then IPM provides people with alternatives.

Usage Scenario

This section will outline how a user can find the information they need using the database. After speaking to NPIC Pesticide Specialists, they hope that users will access this database when asking questions regarding which pesticide to use when comparing two or more, the use of pesticide around a well or other water source, and to find specific physiochemical values for a specific AI (this scenario is specific to pesticide specialists). A potential user may call NPIC in search of this information and, now with the database, an NPIC specialist will refer him or her to the Herbicide Properties Tool. Once there, the user will see a list of each AI. There will be an option to view a table similar to the already existing Pesticide Properties Database on the NPIC website with a list of each AI and columns for each physiochemical property and the GUS calculation. The user can click an AI name in either the list or table view to expand its row. This is where the explanations and images will be for each property as well as the movement rating for each soil type. Some of the images will be in graphics interchangeable format, or GIFs, to represent movement. The

different soil types and each property are color-coded. (Appendix B) Each piece of data will have a Reference link next to it that, when clicked, is sends the user to the primary source PDF file and destination where we found it.

REFERENCES

- ¹ Summary of the Federal Insecticide, Fungicide, and Rodenticide Act. (n.d.). Retrieved February 05, 2016, from <http://www.epa.gov/laws-regulations/summary-federal-insecticide-fungicide-and-rodenticide-act>
- ² About Pesticide Registration. (n.d.). Retrieved February 05, 2016, from <http://www.epa.gov/pesticide-registration/about-pesticide-registration>
- ³ Regulations.gov. (n.d.). Retrieved February 05, 2016, from <http://www.regulations.gov/#!/home>
- ⁴ About NPIC. (n.d.). Retrieved February 05, 2016, from <http://npic.orst.edu/about.html>
- ⁵ Vogue, P.A.; Kerle, E.A.; and Jenkins, J.J. 1994. OSU Extension Pesticide Properties Database. <http://npic.orst.edu/ingred/ppdmove.htm> Accessed December 22, 2015
- ⁶ Wauchope, R. D., T. M. Buttler, A. G. Hornsby, P. M. Augustijn-Beckers, and J. P. Burt. 1992. The SCS/ARS/CES pesticide properties database for environmental decision making. *Reviews of Environ. Contamin. Toxicol.* 123:1-155.
- ⁷ Lewis, K.A., Green, A., Tzilivakis, J. and Warner, D. 2015. The Pesticide Properties DataBase (PPDB) developed by the Agriculture & Environment Research Unit (AERU), University of Hertfordshire, 2006-2015. http://sitem.herts.ac.uk/aeru/iupac/docs/Conditions_of_use.pdf
- 2008, February 11. Pesticide List. Retrieved from <http://www.ars.usda.gov/Services/docs.htm?docid=14147>
- 2014, July 10. How to Manage Pests. Pesticides: Water-Related Risks of Active Ingredients. Retrieved from <http://www.ipm.ucdavis.edu/TOX/watertox1.php>.

- ⁸ Pesticide Product Information System (PPIS). (n.d.). Retrieved February 05, 2016, from <http://www.epa.gov/ingredients-used-pesticide-products/pesticide-product-information-system-ppis>
- ⁹ NPRO. (n.d.). Retrieved February 05, 2016, from <http://npic.orst.edu/NPRO/>
- ¹⁰ Pfeiffer, M. (2010). Groundwater Ubiquity Score (GUS). Retrieved from http://www.ptrpest.com/pdf/groundwater_ubiquity.pdf
- ¹¹ Pesticides Chemical Search | Chemical Search | Pesticides | US EPA. (n.d.). Retrieved February 05, 2016, from <http://iaspub.epa.gov/apex/pesticides/f?p=chemicalsearch:1>
- ¹² Shaner, D.L.. (2014). *Herbicide Handbook*, (Vol. 10). Lawrence, KS: Weed Science Society of America.
- ¹³ 2,4-D EPA EFED Registration Review, page 10 [file:///Users/merrittj/Downloads/EPA-HQ-OPP-2012-0330-0003%20\(1\).pdf](file:///Users/merrittj/Downloads/EPA-HQ-OPP-2012-0330-0003%20(1).pdf)
- ¹⁴ Fernandez-Cornejo, J., Nehring, R., Osteen, C., Wechsler, S., Martin, A., & Vialou, A. (2014, May). Pesticide Use in U.S. Agriculture: 21 Selected Crops, 1960-2008. Retrieved from http://www.ers.usda.gov/media/1424195/eib124_summary.pdf
- ¹⁵ Summary of the Food Quality Protection Act. (n.d.). Retrieved February 05, 2016, from <http://www.epa.gov/laws-regulations/summary-food-quality-protection-act>
- ¹⁶ Pesticide Labels. (n.d.). Retrieved February 05, 2016, from <http://www.epa.gov/pesticide-labels>
- ¹⁷ Pesticides and Pest Management. (2016). Retrieved February 05, 2016, from <http://www.hc-sc.gc.ca/cps-spc/pest/index-eng.php>
- ¹⁸ The Regulations of Pesticides in Canada. (2009). Retrieved February 05, 2016, from http://www.hc-sc.gc.ca/cps-spc/pubs/pest/_fact-fiche/reg-pesticide/index-eng.php

- ¹⁹ An international comparison on Canada's action on pesticide regulation. (n.d.). Retrieved February 05, 2016, from http://www.oag-bvg.gc.ca/internet/English/pet_180_e_28916.html
- ²⁰ Banned or Severely Restricted Pesticides (U.S. Environmental Protection Agency). (n.d.). Retrieved February 05, 2016, from http://scorecard.goodguide.com/chemical-groups/one-list.tcl?short_list_name=brpest
- ECHA. (n.d.). Retrieved February 05, 2016, from <http://echa.europa.eu/web/guest/candidate-list-table>
- ²¹ White Paper on the Strategy for a future Chemicals Policy. (n.d.). Retrieved February 05, 2016, from http://ec.europa.eu/environment/archives/chemicals/reach/background/white_paper.htm?uri=CELEX:52001DC0088
- ²² REACH - Chemicals - Environment - European Commission. (n.d.). Retrieved February 05, 2016, from http://ec.europa.eu/environment/chemicals/reach/reach_en.htm
- ²³ N. (n.d.). Pesticides in Drinking Water. Retrieved July, 2000, from <http://npic.orst.edu/factsheets/drinkingwater.pdf>
- ²⁴ What is Integrated Pest Management (IPM)? (n.d.). Retrieved February 05, 2016, from <http://www.ipm.ucdavis.edu/GENERAL/whatisipm.html>

APPENDICES

Appendix A: Property Descriptions and Factsheets

Property Descriptions

- **Water Solubility**
Water solubility is a measurement of how easily a pesticide dissolves in water. Some mix easily into water while others remain separate.
- **Soil half-life**
Soil half-life is a measurement of how long it takes for a certain amount of a pesticide to be reduced by half while in soil.
- **Sorption coefficient**
Sorption coefficient is a measurement of how well a pesticide will bind to soil particles and organic matter.
- **Hydrolysis half-life**
Hydrolysis half-life is a measurement of how long it takes for a certain amount of a pesticide to be reduced by half while in water.
- **Vapor pressure**
Vapor pressure is a measurement of how likely a chemical is to move into the air as a gas.

Fact Sheets for Half-Life and Water Solubility

<http://npic.orst.edu/factsheets/half-life.html>

<http://npic.orst.edu/envir/watersol.html>

Appendix B: Database Visuals

<http://npic.orst.edu/HPT/index.html>

List View

[Show full table view](#)

Search:

Active Ingredient
1,2-Dibromo-3-chloropropane
1,3-Dichloropropene
2, 4-D, Choline salt
2,4-D
2,4-D 2-ethylhexyl ester
2,4-D butoxyethyl ester
2,4-D dimethylamine salt
2,4-D isooctyl ester
2,4-D isopropyl ester
2,4-D triisopropanolamine salt
2,4-D, diethanolamine salt
2,4-D, isopropylamine salt
2,4-D, methylamine salt
2,4-D, sodium salt

Table View

[Show list view](#)

[Print](#) [Column visibility](#) Search:

Active Ingredient	Water Solubility (mg/L)	Vapor Pressure (mmHg at 25°C)	Hydrolysis Half-life (days)	K _{oc} : Unknown	Half-life: Unknown	GUS: Unknown
1,2-Dibromo-3-chloropropane	1230.000	0.8				
1,3-Dichloropropene	2500.000	34.0	13.5	31		
2, 4-D, Choline salt	569.000	0.00000014	stable			
2,4-D	569.000	0.00000014	stable			
2,4-D 2-ethylhexyl ester	0.087	0.000002				
2,4-D butoxyethyl ester		0.0000045				
2,4-D dimethylamine salt	729000.000	0.00000000079				
2,4-D isooctyl ester		0.000002				
2,4-D isopropyl ester		0.000046				
2,4-D triisopropanolamine salt						
2,4-D, diethanolamine salt						
2,4-D, isopropylamine salt						
2,4-D, methylamine salt		0.00000000089				
2,4-D, sodium salt						
2,4-DB, dimethylamine salt	46.000	0.000071	stable	20	24.5	3.75

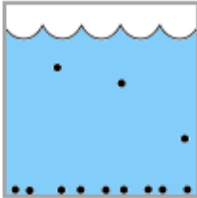
When an AI name is clicked, the following pops up:

2,4-DB, dimethylamine salt ✕

CAS #: 2758-42-1


Water Solubility:

2,4-DB, dimethylamine salt is moderately soluble in water (46.000mg/L)¹.



Vapor Pressure:

2,4-DB, dimethylamine salt will volatilize or become a vapor; some will not (0.000071 mmHg at 25°C)². Increasing heat is likely to make more vapor.




Close

Hydrolysis Half Life:

2,4-DB, dimethylamine salt doesn't break down in water very well. This property is associated with long-term persistence if the chemical reaches groundwater.³

K_{oc}

Unknown soil type:



2,4-DB, dimethylamine salt will not bind to soil particles(20)⁴.

Soil Half Life:

Unknown soil type:

24.5 days⁵

GUS

Unknown soil type:



2,4-DB, dimethylamine salt is likely to move in unknown soils.

Pesticide movement in soil depends on many factors. The more organic matter, the more slowly things tend to move. Compost is high in organic matter, while sand is not. The pesticide's ability to dissolve in water is also very important. For more information, check the "Environmental

TABLES

Table 1. Qualitative benchmarks for Selected Physical/Chemical Properties

Water Solubility	
Source: Ney, Ronald, "Fate and Transport of Organic Chemicals in the Environment" 1995; p. 10	
<10 ppm (mg/L)	(active ingredient) is not very soluble in water. It doesn't dissolve very well.
10-1000 ppm (mg/L)	(active ingredient) is moderately soluble in water.
>1000 ppm (mg/L)	(active ingredient) is very soluble in water. It will dissolve easily.
Vapor Pressure	
Source: Source: Ney, Ronald, "Fate and Transport of Organic Chemicals in the Environment" 1995; p. 19	
< 0.000001 mmHg at 25°C, also expressed 1.0 X 10 ⁻⁶	(active ingredient) is not very likely to volatilize or become a vapor.
0.000001 – 0.01 mmHg at 25°C	Some (active ingredient) will volatilize or become a vapor; some will not. Increasing heat is likely to make more vapor.
>0.01 mmHg at 25°C	(active ingredient) easily becomes a vapor, especially as temperatures rise.
Hydrolysis Half-Life	
Source: US EPA Design for the Environment Program – Version 2.0 August 2011; Table A2. Environmental Toxicity and Fate	
(value) in days < 16	(active ingredient) can be broken down quickly by water.
(value) in days 16-180	When water is present, the amount of (active ingredient) is reduced by 50% every (value) days.
"Stable"	(active ingredient) is not broken down by water. This property is associated with long-term groundwater contamination.
Sorption Coefficient (K_{oc})	
Source: Ney Jr., R. E. <i>Fate and Transport of Organic Chemicals in the Environment: A Practical Guide</i> , 2nd ed.; Government Institutes, Inc.: Rockville, MD, 1995 p. 20.	
<1000	(active ingredient) will not bind to soil particles.
100 –10,000	Some (active ingredient) will bind to soil particles, but not all of it. More (active ingredient) will bind to rich soil compared to sandy soils.
>10,000	(active ingredient) will bind to soil particles strongly. This property slows down or stops movement in soil.

Table 2. Movement Score based on the GUS value.

When only one GUS is calculated...		
< 0.1	(active ingredient) is extremely unlikely to move in the soil profile.	Image for extremely low GUS – apply color filter that matches soil type
0.1 – 2.0	(active ingredient) is unlikely to move in the soil profile.	Image for low GUS – apply color filter that matches soil type
2.0 – 3.0	(active ingredient) has a moderate potential to move in the soil profile.	Image for moderate GUS – apply color filter that matches soil type
3.0 – 4.0	(active ingredient) is likely to move in the soil profile.	Image for high GUS – apply color filter that matches soil type
> 4.0	(active ingredient) is very likely to move in the soil profile.	Image for extremely high GUS – apply color filter that matches soil type