Studying The Fate of 1,4-dioxane in The Environment from Surfactants

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Abstract: *1,4-Dioxane is a colorless liquid organic ether mixture used as a solvent in industry (especially for degreasing), laboratories, and as a stabilizer in chlorinated solvents. Although not a direct ingredient, it appears as an unwanted by-product in the production of ingredients in cosmetics (shampoos, soaps), detergents and other products, forming during the ethoxylation process (PEG compounds). 1,4-Dioxane is highly soluble in water, highly flammable, and is considered a potential carcinogen requiring regulatory control. The aim of the present study was to predict the likely environmental fate of 1,4-dioxane from surfactants using in silico methods.*

Keywords: *surfactants, 1,4-dioxane, environmental fate, in silico methods*

1. AIMS AND BACKGROUND

The fate of 1,4-dioxane from surfactants in the environment is defined by its high mobility and extreme persistence, especially in water and groundwater, where it resists natural degradation [9].

1,4-Dioxane is an unintended byproduct formed during the manufacture of ethoxylated surfactants used in household and personal care products like detergents, shampoos, and cosmetics. It is not an intentionally added ingredient [4, 5]. Many basic cleaning ingredients, such as sodium lauryl sulfate (SLS), can be quite harsh on the skin or have low water solubility. To improve their characteristics (for example, to make them softer, foam better, or act as emulsifiers), manufacturers subject them to a chemical reaction with ethylene oxide (a highly hazardous substance). During this ethoxylation reaction, if the production process is not strictly controlled and optimized, two or more ethylene oxide molecules can react with each other or with other intermediates in an unintended way. This unwanted side reaction leads to the formation of a stable ring compound: 1,4-dioxane. It enters the environment primarily through industrial wastewater discharges, landfill leachates, and the domestic use and subsequent discharge of consumer products into sewage systems. Once in the environment, 1,4-dioxane is highly mobile due to its properties: high water solubility, resistance to degradation and volatility [1, 6, 10, 11]. The high solubility and low volatility of 1,4-dioxane mean that it does not remain "sticky" to soil or readily evaporate from water. Once it enters the soil (for example, from runoff from landfills or industrial sites), it quickly moves downward to groundwater. Unlike many chlorinated solvents (which are denser than water and sink slowly or adsorb to the soil), 1,4-dioxane moves at the same speed as the groundwater itself. This leads to the formation of large, rapidly expanding areas of contamination that are difficult to contain. It is highly resistant to most natural biological and chemical processes in the underground environment, allowing it to persist for decades [2, 3]. 1,4-Dioxane does not accumulate in living organisms. It is readily metabolized and excreted from the bodies of animals and humans, rather than accumulating in fatty tissues (as some other persistent organic pollutants such as pesticides or PCBs do). This means that the risk of contamination through the food chain (for example, through consumption of contaminated fish) is minimal. The main route of exposure for humans is through consumption of contaminated drinking water [7, 8, 12, 13]. The aim of the present study was to predict the likely environmental fate of 1,4-dioxane from surfactants using in silico methods.

2. EXPERIMENTAL

COMPOUND

1,4-Dioxane is a synthetic chemical used primarily as an industrial solvent and stabilizer that is classified as a probable human carcinogen.

It is highly water-soluble and resistant to degradation, making it a common groundwater contaminant and a trace component in some consumer products. 1,4-Dioxane does not occur naturally in the environment, but is an artificially created substance (Fig. 1) [14].

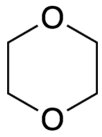


Fig. 1. The structure of 1,4-dioxane

METHODS

The U.S. Environmental Protection Agency's (EPA) CompTox Chemicals Dashboard is an integrated online hub that provides public access to comprehensive data on over 1.2 million chemicals. It is a key tool in the field of computational toxicology and helps scientists and regulators quickly assess potential risks to human health and the environment [15].

3. RESULTS AND DISCUSSION

Due to its unique physicochemical properties – high solubility in water, low vapor pressure, low Henry's Law constant and weak adsorption to organic carbon – 1,4-dioxane cannot be effectively removed by conventional methods such as air stripping, activated carbon filtration or reverse osmosis.

In silico methods are increasingly used to assess the behavior, fate, and risks associated with 1,4-dioxane in the environment. These methods represent computer modeling and simulations that complement or replace traditional laboratory tests (in vitro and in vivo), especially when experimental data are lacking or for a rapid initial assessment. Quantitative Structure-Activity

Relationships (QSAR) and Quantitative Structure-Property Relationships (QSPR) are models that use mathematical relationships to predict the physicochemical properties and biological activity of a given compound based on its molecular structure. For 1,4-dioxane, QSAR/QSPR models help predict key parameters important for its environmental fate.

Using the US Environmental Protection Agency's (EPA) CompTox Chemicals Dashboard database, as well as additional risk assessments, key predictions and findings were made regarding the fate and behavior of 1,4-dioxane in the environment (Table 1-6).

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Table 1. Predicting the Atmos. Hydroxylation Rat of 1,4-dioxane.

Atmos. Hydroxylation Rat, cm^3/molecule·sec	
Experimental average	$1.09 \times e^{-11}$
Predicted average	$1.10 \times e^{-11}$
Experimental median	$1.09 \times e^{-11}$
Predicted median	$1.10 \times e^{-11}$
Experimental range	$1.09 \times e^{-11}$
Predicted range	$1.10 \times e^{-11}$

The data in Table 1 present the atmospheric hydroxylation rate constant for 1,4-dioxane. These values are critical to understanding the chemical's atmospheric fate. The presented results show extremely high accuracy of the in silico models compared to the experimental data. The near-perfect agreement between experimental and predicted values confirms that EPA algorithms are reliable tools for risk assessment when direct laboratory measurements are lacking. This reinforces the role of in silico methods as an effective alternative for environmental monitoring.

Table 2. Bioconcentration Factor of 1,4-dioxane.

Bioconcentration Factor, L/kg	
Experimental average	0.541
Predicted average	1.00
Experimental median	0.505
Predicted median	1.00
Experimental range	0.401 to 700
Predicted range	0.501 to 1.50

The data in Table 2 show the Bioconcentration Factor (BCF) of 1,4-dioxane, which measures the tendency of a chemical to accumulate in the tissues of aquatic organisms (fish, plants) relative to its concentration in water.

Both the experimental and predicted values (mean and median) are very low (close to 1 or less than 1). Values below 100 indicate minimal or no tendency to bioaccumulate.

The predicted mean and median values are in the same order as the experimental ones and indicate that the in silico models accurately predict the low bioaccumulation potential of 1,4-dioxane.

The low BCF indicates that 1,4-dioxane does not pose a significant risk to ecosystems through bioaccumulation or biomagnification (accumulation up the food chain). This result is consistent with the other properties of 1,4-dioxane – it is highly water-soluble and does not readily bind to organic materials (neither in soil nor in living organisms). It prefers to remain dissolved in water.

In summary, in silico BCF models are robust for 1,4-dioxane and confirm that the main environmental threat from this compound is not toxicity through accumulation, but rather contamination of large volumes of drinking water and groundwater due to its extreme mobility and resistance to degradation.

Table 3. Biodeg. Half-Life of 1,4-dioxane

Biodeg. Half-Life, days	
Experimental average	-
Predicted average	9.33
Experimental median	-
Predicted median	9.33
Experimental range	-
Predicted range	9.33

Table 3 presents predictions for the biodegradation half-life of 1,4-dioxane. The lack of experimental data ("-") highlights the usefulness of in silico models to fill information gaps in the evaluation of novel or difficult-to-study compounds. A half-life of about 9 days under ideal (predicted) conditions suggests that 1,4-dioxane does not degrade instantaneously. In natural environments where conditions are not optimal (e.g., in cold, anaerobic groundwater), this half-life can be many times longer, potentially hundreds of days or even years. These data support the general conclusion that 1,4-dioxane is a persistent pollutant. Its natural decay in most environmental environments is a slow process. The use of in silico models in CompTox Dashboard allows rapid assessment of potential biodegradation rates even without experimental data, guiding engineers and regulators towards the implementation of more reliable treatment methods.

Table 4. Fish Biotrans. Half-Life (Km) of 1,4-dioxane.

Fish Biotrans. Half-Life (Km), days	
Experimental average	-
Predicted average	0.162
Experimental median	-
Predicted median	0.162
Experimental range	-
Predicted range	0.162

The data in Table 4 show the half-life of biotransformation (metabolism) of 1,4-dioxane in fish predicted using in *silico* models in the CompTox Chemicals Dashboard. The lack of experimental data once again highlights the importance of computer models for toxicological risk assessment. A half-life of only 0.162 days (approximately 4 hours) is very short. This means that once 1,4-dioxane is ingested or absorbed, aquatic organisms process and eliminate it from their bodies within a few hours. This rapid metabolism (biotransformation) is the main reason for the low bioconcentration factor (BCF) discussed in Table 2. The substance fails to accumulate in tissues because it is broken down faster than it is absorbed. From an ecotoxicological perspective, this prediction is a positive sign. Acute toxic effects on aquatic organisms through accumulation are unlikely. The risk is more likely to be associated with chronic exposure to high concentrations in the aquatic environment than with bioaccumulation along the food chain. The CompTox Dashboard data, although in *silico* predictions, provide a strong indication that 1,4-dioxane does not pose a threat through accumulation in living matter. The main concern remains its mobility in water resources and its difficulty in removal by standard treatment methods.

Table 5. Ready Binary Biodegradability of 1,4-dioxane.

Ready Binary Biodegradability, binary (0/1)	
Experimental average	-
Predicted average	1.00
Experimental median	-
Predicted median	1.00
Experimental range	-
Predicted range	1.00

The data in Table 5 present the results of the binary test for "Ready Biodegradability", which is a standard screening test (OECD 301). In these tests, a score of "1" means that the substance is considered "readily biodegradable" (it reaches a certain degradation threshold, usually above 60% in 28 days, under laboratory conditions with an inoculum of microorganisms). A score of "0" means that it does not degrade readily. The predicted score of "1.00" suggests that the *in silico* model expects 1,4-dioxane to pass the test for ready biodegradation under ideal laboratory conditions. This predicted result seems contradictory to the common understanding and experimental data that 1,4-dioxane is a persistent pollutant that is difficult to degrade in the natural environment. "Ready Biodegradability" tests provide optimal conditions - high concentrations of oxygen, nutrients and adapted microorganisms. In these artificial conditions, the *in silico* model correctly predicts that if the specific enzymes are present, degradation is possible. The model can predict degradation potential based on structure, but cannot account for the presence of the appropriate microbial community in a given real-world environment. The prediction from Table 5 confirms that 1,4-dioxane is susceptible to biodegradation under the right conditions and the presence of specific microorganisms. This reinforces the conclusion that bioremediation through bioaugmentation (addition of specialized bacteria) is a viable treatment technology, although in most natural conditions it remains a persistent and highly mobile pollutant.

Table 6. Soil Adsorp. Coeff (Koc) of 1,4-dioxane.

Soil Adsorp. Coeff (Koc), L/kg	
Experimental average	17.0
Predicted average	17.0
Experimental median	17.0
Predicted median	17.0
Experimental range	17.0
Predicted range	17.0

The data in Table 6 show the adsorption coefficient to soil organic carbon for 1,4-dioxane. The complete agreement between the experimental and predicted values (17.0 L/kg) confirms the high accuracy of the EPA models for this property. The coefficient (Koc) measures the tendency of a chemical to bind to organic matter in soil. A value of 17.0 L/kg is considered extremely low on the international mobility scales (where values below 50 are defined as "very mobile"). Due to its low affinity for soil particles, 1,4-dioxane is hardly retained in the soil matrix. It remains dissolved in the aqueous phase. In summary, the Koc data strongly support the definition of 1,4-dioxane as a highly mobile and persistent pollutant whose management requires a focus on water resources rather than soil remediation.

4. CONCLUSIONS

1,4-Dioxane is a substance with a unique set of physicochemical properties that determine its behavior as a challenging and persistent pollutant, especially in water resources. The main environmental risk of 1,4-dioxane is not related to accumulation in the food chain or long-term presence in the air, but to its exceptional ability to contaminate large volumes of drinking water and groundwater due to its high mobility and resistance to conventional treatment methods. This requires the use of specialized and expensive technologies such as Advanced Oxidation Processes (AOP) for its effective removal.

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