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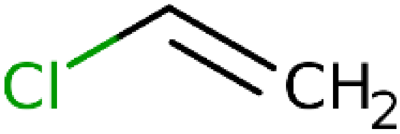
Pollution Prevention

Draft Chemistry and Fate Assessment for Vinyl Chloride

Technical Support Document for the Draft Scope for Vinyl Chloride (Ethene, chloro-)

CASRN 75-01-4



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Docket

Supporting information can be found in the public docket, Docket ID: EPA-HQ-OPPT-2018-0448.

Disclaimer

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This draft technical support document was reviewed and cleared for release by OPPT and OCSPP leadership.

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ABBREVIATIONS AND ACRONYMS

BAF	Bioaccumulation factor
BCF	Bioconcentration factor
BOD	Biological oxygen demand
CASRN	Chemical Abstracts Service Registry Number
CFR	Code of Federal Regulations
COU	Condition of use
CTD	Characteristic travel distance
DCE	Dichloroethylene
DMR	Discharge Monitoring Report
DOC	Dissolved organic carbon
dw	Dry weight
EPA	Environmental Protection Agency
EPI Suite™	Estimation Program Interface Suite™
EPICS	Equilibrium Partitioning in Closed System
ETH	ethene
FR	Federal Register
HCl	Hydrochloric acid
HLC	Henry's Law constant
HSDB	Hazardous Substances Data Bank
Log K_{AW}	Logarithmic air:water partition coefficient
Log K_{DOC}	Logarithmic dissolved organic carbon:water partition coefficient
Log K_{OA}	Logarithmic octanol:air partition coefficient
Log K_{OC}	Logarithmic organic carbon:water partition coefficient
Log K_{OW}	Logarithmic octanol:water partition coefficient
Log K_{SW}	Logarithmic soil:water partition coefficient
LOQ	Limit of quantification
LRTP	Long-range transport potential
MCL	Maximum contaminant level
MDL	Method detection limit
MOCLA	Model for Organic Chemicals in Landfills
ND	Non-detect/not detected
OC	Organic carbon
OECD	Organisation for Economic Co-operation and Development
·OH	Hydroxyl radical
PCE	Perchloroethylene
P_{OV}	Overall persistence
ppm	parts per million
PVC	Polyvinyl chloride
RCRA	Resource Conservation and Recovery Act
SDWA	Safe Drinking Water Act
STP	Sewage treatment plant
$t_{1/2}$	Half-life
TCE	Trichloroethylene
TG	Test guideline
TRI	Toxics Release Inventory
TSCA	Toxic Substances Control Act
U.S.	United States
UV	Ultraviolet

VOC	Volatile organic chemical
WQP	Water Quality Portal
ww	Wet weight
WWTP	Wastewater treatment plant

SUMMARY

Key Points: Physical, Chemical, and Fate Properties

EPA reviewed databases and previously conducted assessments to identify information for physical and chemical properties to characterize vinyl chloride's expected behavior in the environment, including its tendency to persist in the environment or bioaccumulate. Fate and transport information was collected and considered when identifying the major and minor pathways to inform problem formulation, and during preliminary media assessments for the purposes of the draft scope of the risk evaluation for vinyl chloride (U.S. EPA, 2025). The key points are summarized below:

- Vinyl chloride, also known as chloroethylene, is a chlorinated ethene that does not occur naturally in the environment. Its primary use is as a reactant (monomer) in the production of polyvinyl chloride (PVC). Due to its physical state as a gas at room temperature and pressure, vinyl chloride is primarily expected to be found in the air compartment.
- Upward of 98 percent of annual Toxics Release Inventory (TRI) reported vinyl chloride releases are to the air compartment. Vinyl chloride is expected to undergo indirect photolysis in the atmosphere with photochemically produced hydroxyl radicals (•OH; $t_{1/2}$ of 1.27–2.71 days), though it is not expected to undergo direct photolysis as it does not absorb wavelengths above 218 nm.
- Vinyl chloride is not expected to undergo hydrolysis in aqueous environments.
- With a water solubility of 9,150 mg/L at 20.5 °C, vinyl chloride may exist in surface waters from incidental direct releases (*e.g.*, spills from regular handling or transport of vinyl chloride). However, such instances are expected to be localized and irregular.
- Vinyl chloride is not expected to be readily biodegradable under aerobic aqueous conditions, though it is expected to volatilize from surface water as indicated by its Henry's Law constant (0.0278 $\text{atm}\cdot\text{m}^3/\text{mol}$ at 24.8 °C).
- Because of its range of empirical log K_{OC} values (log K_{OC} 1.75–2.95), vinyl chloride is expected to have some affinity to organic material in solids. In aqueous environments, fugacity modeling indicates that vinyl chloride will not accumulate appreciably in sediments.
- Minimal releases of vinyl chloride are to land/soil media. Due to vinyl chloride's vapor pressure (2,550 mm Hg at 20 °C), it is expected to volatilize from dry soil. However, in areas of incidental, direct releases to land (*e.g.*, spills, leaks), vinyl chloride may also be subject to migration to groundwater, with possible biodegradation and sorption to organic solid fractions.
- Vinyl chloride may be produced in anaerobic environments (*e.g.*, groundwater, landfills) by the reductive dehalogenation of other chlorinated solvents, namely perchloroethylene (PCE) and trichloroethylene (TCE). However, it is unlikely for vinyl chloride to appear in groundwater and landfills from the conditions of use identified in this draft scope.
- The removal of vinyl chloride in wastewater treatment is expected to be primarily by stripping to air (volatilization). Biodegradation is not expected to be a significant removal process. Because of its tendency to volatilize rather than sorb to organic matter, transfer to soil through biosolid amendments or to landfills by sludge disposal is not expected to be a major pathway.
- Vinyl chloride is not expected to bioconcentrate or bioaccumulate significantly in aquatic organisms (BCF = 40 in green algae (*Chlorella fusca*) and BCF < 10 in golden ide (*Leuciscus idus melanotus*)). No bioconcentration or bioaccumulation data were identified for terrestrial organisms.

1 INTRODUCTION

Vinyl chloride, also referred to as chloroethylene, belongs to the chlorinated ethene group that also includes other chlorinated solvents such as perchloroethylene (PCE) and trichloroethylene (TCE). Vinyl chloride does not occur naturally in the environment. It is produced by either oxychlorination or direct chlorination of ethylene to produce 1,2-dichloroethane, followed by thermal cracking of 1,2-dichloroethane to yield vinyl chloride and hydrogen chloride (HCl) (ATSDR, 2024; Cowfer and Gorensek, 2006). The vast majority of vinyl chloride is used in the production of polyvinyl chloride (PVC) and its copolymers (ATSDR, 2024).

Vinyl chloride is a colorless gas at room temperature and pressure (NLM, 2023b; RSC, 2023; U.S. EPA, 2000) and has a boiling point of –13.9 °C (NLM, 2023b; Reaxys, 2023; U.S. EPA, 2023). Vinyl chloride has a water solubility of 9,150 mg/L at 20.5°C (ECHA, 2023a; Reaxys, 2023), a vapor pressure of 2,550 mmHg (ECHA, 2023a) at 20 °C, and a Henry’s Law constant (HLC) of 0.0278 atm·m^3/mol at 24.8 °C (PhysProp, 2023). Because of its boiling point and volatility, vinyl chloride is primarily expected to be found in the air compartment in gas phase.

2 PHYSICAL AND CHEMICAL PROPERTY ASSESSMENT

2.1 Evidence Integration for Physical and Chemical Properties for Vinyl Chloride

EPA reviewed databases and previously conducted assessments to identify information for physical and chemical properties to characterize vinyl chloride's expected behavior in the environment, including its tendency to persist in the environment or bioaccumulate.

Table 2-1 summarizes the information identified for physical and chemical properties of vinyl chloride. Through implementation of systematic review approaches as described in Sections 4 and 5 of the *Updated Search Strategies Used to Identify Potentially Relevant Discipline-Specific Information* (U.S. EPA, 2024b), EPA identified 225 data sources that contain potentially relevant physical and chemical property information of vinyl chloride. During the draft scoping of vinyl chloride, EPA considered both measured and estimated physical and chemical property data/information. Data obtained from expert and peer-reviewed sources were considered first, namely from the Merck Index, the CRC Handbook of Chemistry and Physics, and PubChem HSDB. Additionally, data collected using established test guidelines (*e.g.*, as established by OECD) were prioritized over those not collected following guidelines. EPA selected empirical and measured data over modeled data as much as possible to improve the confidence in the endpoints.

A composite plot consisting of box and whisker plots of reported physical and chemical property data values is shown in Figure 2-1. For some temperature-dependent physical and chemical properties (*e.g.*, vapor pressure, density), the data presented in Figure 2-1 includes measurements collected at temperatures beyond standard environmental conditions (*i.e.*, 20 to 25 °C and 760 mmHg), contributing to the illustrated variance. The box and whisker plots for each endpoint illustrate the mean (average, indicated by the blue diamond) and the 10th, 25th, 50th (median), 75th, and 90th percentiles. All individual data points are indicated by black circles, and the value preliminarily selected for use in the draft scope is overlaid (indicated by the orange star) to provide context for where it lies within the distribution of the data set. Additionally, note that the y-axis scales in each of the panels of Figure 2-1 are different, therefore selected values that appear to be far from the central tendency of the data set may in fact be numerically in close agreement (*e.g.*, log K_{OW}, vapor density, and density). The data included for each of the displayed endpoints in Figure 2-1 are described in respective preliminary endpoint assessment sections, beginning in Section 2.1.2.

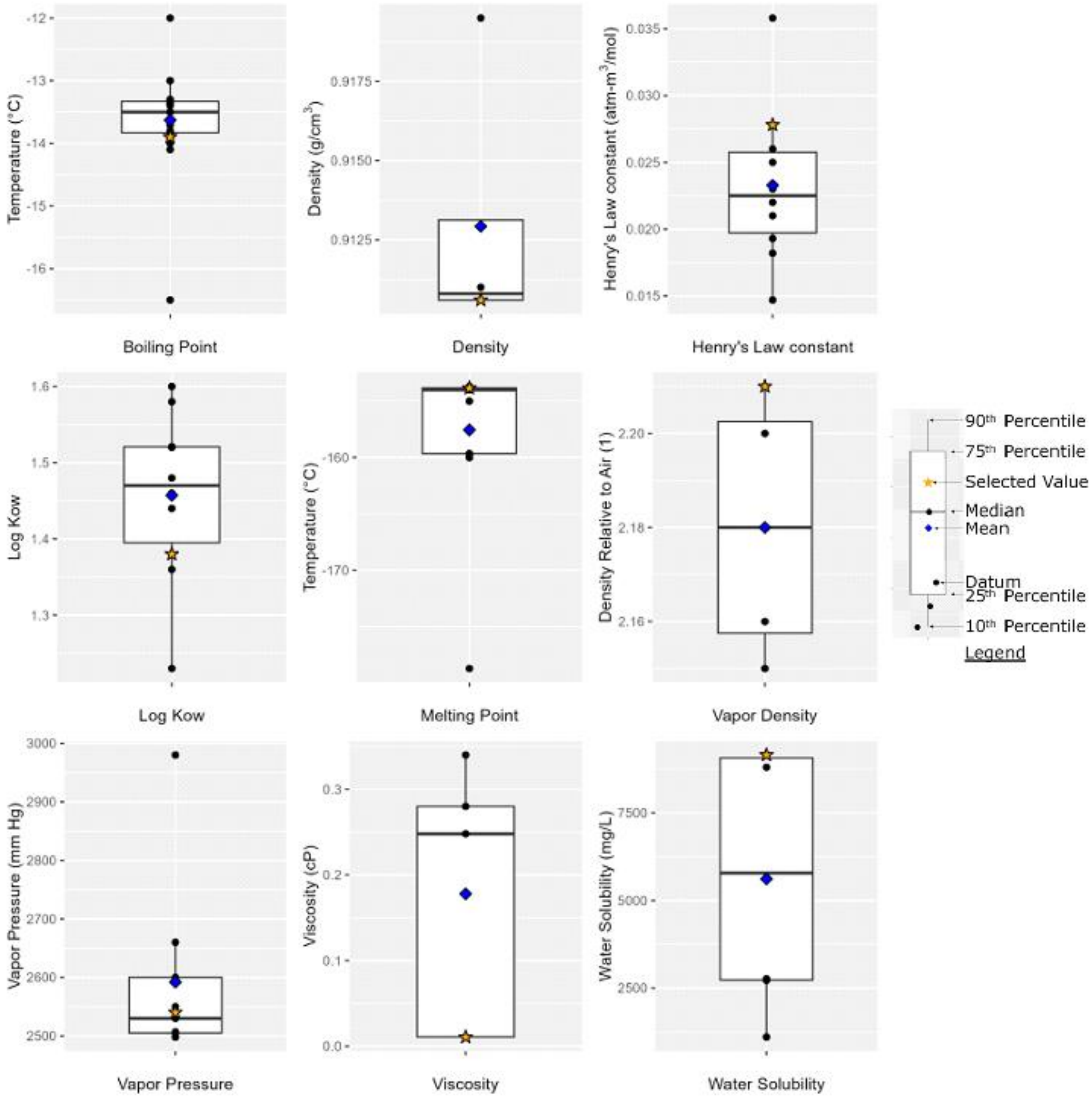


Figure 2-1. Box and Whisker Plots of Reported Physical and Chemical Property Data Values and Preliminarily Selected Values for Vinyl Chloride

2.1.1 Preliminarily Selected Physical and Chemical Property Values for Vinyl Chloride

For some physical and chemical properties, there are multiple high-confidence values available for selection that were identified. The majority of the preliminarily selected data were collected under standard environmental conditions (*i.e.*, 20–25 °C and 760 mmHg). For values of endpoints for which no empirical data were identified, estimations from EPI Suite™ are reported (U.S. EPA, 2017).

Table 2-1. Physical and Chemical Properties of Vinyl Chloride

Property	Selected Value[a]	Reference(s)
Molecular formula	C_2H_3Cl	NLM (2023b)
Molecular weight	62.498 g/mole	Rumble (2023)
Physical form	Colorless gas at room temperature and pressure; mild, sweet odor	RSC (2023), U.S. EPA (2000), NLM (2023b)
Melting point	–153.84 °C	PhysProp (2023), Rumble (2023)
Boiling point	–13.9 °C	NLM (2023b), U.S. EPA (2023), Reaxys (2023)
Density	0.9106 g/cm^3 at 20 °C	Rumble (2023), RSC (2023), ATSDR (2024), OECD (2001)
Vapor pressure	2,550 mm Hg at 20 °C	ECHA (2023a)
Vapor density	2.21 (relative to air = 1)	NLM (2023b)
Water solubility	9,150 mg/L at 20.5 °C	Reaxys (2023), ECHA (2023a)
Octanol:water partition coefficient (log K_{OW})	1.38	Rumble (2023), ATSDR (2024), ECHA (2023c)
Octanol:air partition coefficient (log K_{OA})	1.324[b]	EPI Suite™ (KOAWIN)
Henry's Law constant	0.0278 atm·m^3/mol at 24.8 °C	PhysProp (2023)
Flash point	–78 °C (closed cup)	NLM (2023b), RSC (2023)
Autoflammability	472 °C	NLM (2023b)
Viscosity	0.01072 cP at 20 °C	NLM (2023b)
UV-Vis absorption	Chemical is a gas that does not absorb wavelengths >218 nm	OECD (2001), ATSDR (2024)

[a] Measured unless otherwise noted
[b] Information was estimated using EPI Suite™ U.S. EPA (2017).

2.1.2 Preliminary Endpoint Assessments

The physical and chemical property values selected preliminarily and for use in this draft scope of vinyl chloride are given in Table 2-1. Data from expert and peer-reviewed databases and reference texts were favored during the selection of preliminarily proposed physical and chemical properties, as discussed in Section 2.1. Because a systematic workflow was used to obtain these data, the data analyses consider only a subset of all physical and chemical data, not an exhaustive acquisition of all potential data. Due to cross-referencing between many of the databases identified and assessed through the systematic review process, there is potential for data from one primary source to be collected multiple times resulting in duplication within the data set. This duplication should be considered as a potential source of uncertainty in the data analyses (*e.g.*, calculation of quartiles presented in Figure 2-1), although data-collection procedures and expert judgement were used to minimize this possibility whenever possible. Additional information may be considered in subsequent analyses after the completion of the systematic review process during the development of the final scope and risk evaluation of vinyl chloride. However, the preliminary selections of physical and chemical properties for vinyl chloride are not expected to change significantly with the completion of the formal systematic review, as many of the same sources are likely to be captured.

2.1.2.1 Molecular Formula, Molecular Weight, and Physical Form

The molecular formula for vinyl chloride is C_2H_3Cl, as presented in NLM (2023b). Four sources for vinyl chloride's molecular weight were identified, and are all in close agreement: ATSDR (2024) and Merck (2023) both provide a molecular weight of 62.50 g/mol. Rumble (2023) reported a molecular weight of 62.948 g/mol, while a molecular weight of 62.9488 g/mol was reported by Reaxys (2023). The value of 62.948 g/mol was selected for this draft scope, as values from the CRC Handbook of Chemistry and Physics are reviewed by subject matter experts and are routinely updated (Rumble, 2023).

Twenty-five values for physical form were identified. The physical form description presented in Table 2-1 represents the most common descriptors identified among the retrieved data, again prioritizing information gathered from expert and/or peer-reviewed trusted databases.

2.1.2.2 Melting Point

Melting point informs the chemical's physical state, environmental fate and transport, as well as the chemical's potential bioavailability. After data set deduplication, thirteen melting point data values were considered for vinyl chloride, ranging from –178.72 (NIST, 2023) to –153.7 °C (ECHA, 2023b), with a median of –154 °C. A melting point value of –153.84 °C was preliminarily selected for the purposes of this draft scope, as it is in close agreement with the median of the identified melting point data set and was reported by a preferred database reference (the CRC Handbook of Chemistry and Physics; (Rumble, 2023; PhysProp, 2023)). Note that all thirteen data values are presented in Figure 2-1.

2.1.2.3 Boiling Point

Boiling point informs the chemical's physical state, environmental fate and transport, as well as the chemical's potential bioavailability. After deduplication of the boiling point data set, twenty-four boiling point values were considered for vinyl chloride, ranging from –33.51 (NIST, 2023) to 82.7 °C (ECHA, 2023b). Three of the identified values listed in (Reaxys, 2023) are positive (>0 °C) and were thus excluded as outliers. Two additional values were excluded from consideration because they were collected under reduced pressures, and thus are not informative for scenarios under environmental conditions (Reaxys, 2023). The remaining nineteen values are presented in Figure 2-1 and fall between –18 and –12 °C (Reaxys, 2023). A boiling point of –13.9 °C was preliminarily selected for this draft scope as it falls close to the central tendency of identified values (mean of –13.63 °C) and was reported by several high-quality trusted databases (NLM, 2023b; Reaxys, 2023; U.S. EPA, 2023).

2.1.2.4 Density

After deduplication of the data set, twenty density values were considered for vinyl chloride ranging from 0.822 to 2.598 g/cm^3, collected at temperatures ranging from –30 to 64.1 °C. The maximum of the data (2.598 g/cm^3) was excluded as it is a clear outlier (OECD, 2001). Of the remaining nineteen values, four density values were collected at 20 °C, of which the median density is 0.9108 g/cm^3 (ECHA, 2023c; NLM, 2023b; Reaxys, 2023; OECD, 2001). Figure 2-1 presents only the density values collected at 20 °C for the density of vinyl chloride to display values collected at an environmentally relevant temperature, as the other fifteen values were collected under temperatures not reflective of typical environmental conditions. A value of 0.9106 g/cm^3 at 20 °C was preliminarily selected for use in this draft scope as it falls close to the median of density values collected at 20 °C and was also reported by several high-quality trusted reference texts and existing assessments (ATSDR, 2024; RSC, 2023; Rumble, 2023; OECD, 2001).

2.1.2.5 Vapor Pressure

Vapor pressure indicates a chemical's potential to volatilize, affecting the chemical's proneness for fugitive and other emissions to air and for undergoing long range transport. After deduplication, thirty values were considered for the vapor pressure of vinyl chloride, reported at a range of temperatures: from 1 mmHg at –109.4 °C, to 7,603 mmHg at –28.8 to 60.2 °C (Reaxys, 2023). Because vapor pressure measurements are particularly sensitive to temperature, experimental temperature was used to narrow down the selection. The remaining 21 values were excluded: two identified values did not have associated temperatures (NLM, 2023b), one value was presented for a wide range of temperatures (Reaxys, 2023), and the remaining values were collected at temperatures outside of the standard range (*i.e.*, 20-25 °C). Six of the thirty values were collected at 20 °C with a mean of 2,515 mmHg (ATSDR, 2024; ECHA, 2023a, c; NLM, 2023b; PhysProp, 2023; RSC, 2023; OECD, 2001), while three were collected at 25 °C with a mean of 2,747 mmHg (ATSDR, 2024; PhysProp, 2023; Rumble, 2023; U.S. EPA, 2000). Figure 2-1 presents only the data collected at 20 °C or 25 °C for the vapor pressure of vinyl chloride. A vapor pressure of 2,550 at 20 °C was preliminarily selected for use in this draft scope as it is representative of vinyl chloride's vapor pressure under environmentally relevant conditions (ECHA, 2023a).

2.1.2.6 Vapor Density

Four values were identified for the vapor density of vinyl chloride ranging from 2.15 to 2.21 (relative to air = 1), all in close agreement (ATSDR, 2024; NLM, 2023a, b). A vapor density of 2.21 was preliminarily selected for use in this draft scope as it was reported by a preferred database (NLM, 2023a, b).

2.1.2.7 Water Solubility

Water solubility informs many endpoints not only within the realm of fate and transport of vinyl chloride in the environment, but also when modelling for industrial process, engineering, human and ecological hazard, and exposure assessments. Nineteen data were identified for the water solubility of vinyl chloride ranging from 1,000 to 9,950 mg/L collected at 15 to 80 °C (ECHA, 2023a; Reaxys, 2023). Six water solubility values were collected at temperatures between 20 and 25 °C and are presented in Figure 2-1. The other thirteen values were excluded from consideration as they were not collected under standard environmental temperature. A water solubility of 9,150 mg/L at 20.5 °C was preliminarily selected for use in this draft scope as it was reported by multiple high-quality references and was collected at a temperature representative of relevant environmental conditions (ECHA, 2023a; Reaxys, 2023).

2.1.2.8 Octanol:Water Partition Coefficient (log K_{OW})

The octanol:water partition coefficient (log K_{OW}) quantifies how a chemical will partition between octanol (a common surrogate for biological lipids and other hydrophobic media) and water. In the absence of adequate empirical data, log K_{OW} is often used to predict a chemical's tendency to partition to biota (*i.e.*, bioconcentration), as well as for the estimation of other properties including water solubility, soil adsorption, and bioavailability. After deduplication, ten log K_{OW} values were considered for vinyl chloride. All identified values are in good agreement, falling between 1.23 and 1.6 (ATSDR, 2024; NLM, 2023b). The small variance in the log K_{OW} data set for vinyl chloride increases confidence that the selected value is representative of vinyl chloride octanol:water partitioning. The value 1.38 collected at 20 °C and pH 5 to 9 was preliminarily selected for use in this draft scope, as this value was collected following OECD Guideline 107 and was reported by several high-quality databases and existing evaluations (ATSDR, 2024; ECHA, 2023c; Rumble, 2023). All ten values are presented in Figure 2-1.

2.1.2.9 Octanol:Air Partition Coefficient (log K_{OA})

No empirical log K_{OA} data were identified from the screening of databases and previously released assessments. The EPI Suite™ KOAWIN model was leveraged to estimate a log K_{OA} of 1.324 (U.S. EPA, 2017).

2.1.2.10 Henry's Law Constant

The Henry's Law constant (HLC) provides an indication of a chemical's volatility from water and gives an indication of environmental partitioning between air and water, potential removal during wastewater treatment via aeration stripping, and possible routes of environmental exposure. After deduplication, thirteen HLC values were considered for vinyl chloride ranging from 0.0147 to 1.05 atm·m^3/mol. Values increased with temperature, with reported values collected at conditions of 9.85 to 34.6 °C. Three values (0.055, 0.12, and 1.05 atm·m^3/mol) were excluded from consideration as statistical outliers (NIST, 2023); the remaining ten values fall between 0.0147 to 0.0358 atm·m^3/mol. The value 0.0278 atm·m^3/mol at 24.8 °C was preliminarily selected for use in this draft scope as it was collected using the equilibrium partitioning in closed system (EPICS) method often employed for VOCs, it was collected close to standard temperature, and was reported by multiple databases and existing assessments (ECHA, 2023a; PhysProp, 2023). Because the selected value is the only HLC value for which the collection temperature could be confirmed as environmentally relevant, all eleven HLC values remaining after removing outliers are presented in Figure 2-1 to illustrate the data set variance. This explains why the selected HLC value lies above the central tendency, as values collected below standard temperature are smaller than those collected at standard temperature.

2.1.2.11 Flash Point and Autoflammability

Limited data were identified for the flash point and autoflammability of vinyl chloride. The flash point value of –78 °C (determined by the closed cup method) was reported by both (NLM, 2023b) and (RSC, 2023), and was preliminarily selected for use in this draft scope. Similarly, an autoflammability of 472 °C was selected for use in this draft scope (NLM, 2023b).

2.1.2.12 Viscosity

Four references were identified reporting the viscosity of vinyl chloride, ranging from 0.01072 to 0.34 cP within a temperature range of –40 °C to 30 °C (NLM, 2023a, b; Reaxys, 2023). Under relevant environmental conditions, vinyl chloride will exist as a gas with a viscosity of 0.01072 cP (collected at 20 °C) (NLM, 2023a, b). As a liquid at –20 °C, vinyl chloride has a viscosity of 0.280 cP (NLM, 2023a, b); these values were preliminarily selected to represent gas and liquid phase viscosities of vinyl chloride. Note that Figure 2-1 presents all viscosity data identified.

2.1.2.13 UV-Vis Absorption

The UV-Vis absorption range and maxima of a chemical indicate whether or not the chemical may be susceptible to direct photolysis in the atmosphere. Both (OECD, 2001) and (ATSDR, 2024) reported the absorption range of vinyl chloride to fall below 218 nm, suggesting vinyl chloride is not susceptible to direct photolysis.

3 ENVIRONMENTAL FATE AND TRANSPORT ASSESSMENT

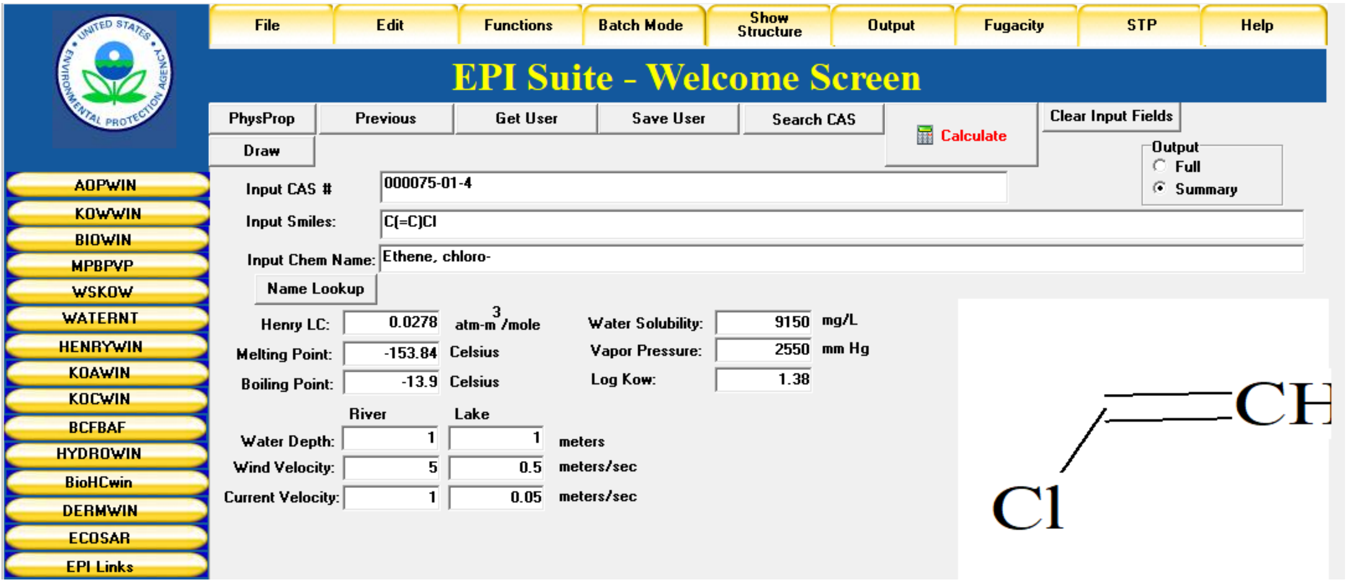
3.1 Approach and Methodology

EPA reviewed databases and previously conducted assessments to identify information on fate endpoints for vinyl chloride that inform fit-for-purpose risk evaluation analysis plans (see Section 3.2 of the *Updated Search Strategies Used to Identify Potentially Relevant Discipline-Specific Information* (U.S. EPA, 2024b)). Specifically, this information was analyzed to characterize transport and partitioning pathways, identify environmental persistence potential, and assess bioaccumulation potential of vinyl chloride. EPA conducted a Tier I assessment to identify the environmental compartments (*i.e.*, water, sediment, biosolids, soil, groundwater, air) of major and minor relevance to the fate and transport of vinyl chloride as indicated by its partitioning behavior. Next, a Tier II fugacity analysis was conducted to preliminarily inform the fate pathways and media most likely to result in exposure from environmental releases to inform which media should be the focus of quantitative vs. qualitative assessments. The Tier II analysis was performed using EPI Suite^{TM} (LEV3EPI^{TM}) as described in Section 3.1.1 (U.S. EPA, 2017). The results of the Tier I and II assessments are discussed in Section 3.2.

Complementing preliminary Tier I and Tier II analyses, understanding the transformation behavior of vinyl chloride informs which pathways are expected to be dominant or contributing to persistence in different compartments. Vinyl chloride undergoes various transformation processes as discussed in Section 3.3. Last, EPA preliminarily assessed the environmental fate and transport of vinyl chloride by considering and integrating physical and chemical data, fate and transport data, monitoring data, and release data identified to date. With this, EPA performed preliminary media-specific fate analyses as described in Section 3.3.4.

3.1.1 EPI Suite^{TM} Model Inputs and Settings

To set up EPI Suite™ for estimating fate and fugacity properties of vinyl chloride, the physical and chemical properties were input based on the values in Table 2-1. EPI Suite™ was run using default settings (*i.e.*, no other parameters were changed or input) unless otherwise stated below (Figure 3-1).



Output
○ Full
● Summary

Input CAS #: 000075-01-4
Input Smiles: C(=C)Cl
Input Chem Name: Ethene, chloro-

Henry LC: 0.0278 atm-m^3/mole
Melting Point: -153.84 Celsius
Boiling Point: -13.9 Celsius
Water Solubility: 9150 mg/L
Vapor Pressure: 2550 mm Hg
Log Kow: 1.38

	River	Lake	
Water Depth:	1	1	meters
Wind Velocity:	5	0.5	meters/sec
Current Velocity:	1	0.05	meters/sec

Figure 3-1. Screen Capture of EPI Suite^{TM} Parameters Used to Calculate Physical and Chemical Properties and Environmental Fate for Vinyl Chloride

Fugacity Modeling Sensitivity Analysis

Using a fugacity modeling approach helps to inform how vinyl chloride is expected to be distributed in the environment. The approach described by Mackay (1996) using the Level III Fugacity model in EPI Suite™ (LEV3EPI™) was used for Tier II analysis. LEV3EPI™ is described as a steady-state, non-equilibrium model that uses a chemical's physical and chemical properties and degradation rates to predict partitioning of the chemical between environmental compartments and its persistence in a model environment (U.S. EPA, 2017).

Because systematic review and data quality evaluation steps are not yet complete, a sensitivity analysis was conducted to gauge a range of scenarios by varying compartment half-lives ($t_{1/2}$), and tendency to adsorb to organic carbon (varying log K_{OC}): here, the minimum, mean, and maximum empirical half-lives of vinyl chloride transformation in soil, water, and sediment were assessed, as well as the minimum and maximum log K_{OC} (see Section 3.2.1). Since the reported half-lives of vinyl chloride transformation in air are in relative agreement (mediated by indirect ·OH photolysis; Table 3-2), the mean atmospheric half-life was used in all runs. In instances where transformation half-lives were not available from the identified sources, a first-order approximation was calculated from the fraction of vinyl chloride remaining and the study duration, using the first-order rate equation:

Equation 3-1

$$t_{1/2} = \frac{\ln(2)}{-\ln(f_{VC_{remain}})/t}$$

Where:

$t_{1/2}$ = half-life (hours)
f_{VC_remain} = fraction of vinyl chloride remaining at time t
t = study duration (hours)

The studies used and their calculated half-lives are presented in Appendix A in further detail. In addition to the half-life and log K_{OC} sensitivity bounding, two sets of different release scenarios were screened to assess how direct releases to specific compartments affect the overall mass distribution in the fugacity model. The two sets of release values used as inputs to the fugacity model are described below.

The first set was run using the mean reported releases (kg/hr) submitted to TRI over the past ten years. The TRI information on releases to the environment are presented in the *Proposed Designation of Vinyl Chloride as a High-Priority Substance for Risk Evaluation* (U.S. EPA, 2024a). In summary, of the more than 5 million lb of vinyl chloride disposed of or otherwise released to the environment during the TRI reporting years 2013 through 2022, more than 98 percent was released onsite to air. The majority of offsite releases reported to TRI were to wastewater treatment facilities other than publicly owned treatment works (*e.g.*, industrial wastewater treatment). TRI releases that were categorized as RCRA landfill releases were not included in the land releases, as environmental releases from RCRA landfills (*e.g.*, through leachate runoff) were assumed to be negligible.

The second set probed generic release scenarios to single compartments to inform the fugacity tendencies of vinyl chloride in each media. A summary of the inputs for each LEV3EPI™ run is listed in Table 3-1. Bolded values in the rows of Table 3-1 indicate which value was adjusted to test the sensitivity of the associated parameter (*i.e.*, half-life or K_{OC}).

Table 3-1. Summary of Vinyl Chloride Parameters Inputted for EPI Suite™ Level III Fugacity Sensitivity Analysis

Release Source	Run No.	Releases (kg/hr)			K_{OC}[a]	Half-Lives ($t_{1/2}$; hours)[a]				Run Notes
		Air	Water	Soil		Air	Water	Soil	Sediment	
TRI RELEASES	1	2.6E+01	2.8E-03	1.4E-04	56.2	44.3	1630	763.6	1778	min K_{OC}; mean water, soil, and sediment $t_{1/2}$
	2	2.6E+01	2.8E-03	1.4E-04	**891.3**	44.3	1630	763.6	1778	max K_{OC}; mean water, soil, and sediment $t_{1/2}$
	3	2.6E+01	2.8E-03	1.4E-04	56.2	44.3	2672	763.6	1778	min K_{OC}, max water $t_{1/2}$
	4	2.6E+01	2.8E-03	1.4E-04	56.2	44.3	**344**	763.6	1778	min K_{OC}, min water $t_{1/2}$
	5	2.6E+01	2.8E-03	1.4E-04	56.2	44.3	1630	**1711.4**	1778	min K_{OC}, max soil $t_{1/2}$
	6	2.6E+01	2.8E-03	1.4E-04	56.2	44.3	1630	**195.1**	1778	min K_{OC}, min soil $t_{1/2}$
	7	2.6E+01	2.8E-03	1.4E-04	56.2	44.3	1630	763.6	**12000**	min K_{OC}, max sediment $t_{1/2}$
	8	2.6E+01	2.8E-03	1.4E-04	56.2	44.3	1630	763.6	**21.7**	min K_{OC}, min sediment $t_{1/2}$
"GENERIC" RELEASES [b]	9	1000	1000	1000	56.2	44.3	1630	763.6	1778	min K_{OC}, equal releases
	10	1000	1000	1000	**891.3**	44.3	1630	763.6	1778	max K_{OC}, equal releases
	11	0	1000	0	56.2	44.3	1630	763.6	1778	min K_{OC}, water releases only
	12	0	1000	0	**891.3**	44.3	1630	763.6	1778	max K_{OC}, water releases only
	13	0	0	1000	56.2	44.3	1630	763.6	1778	min K_{OC}, soil releases only
	14	0	0	1000	**891.3**	44.3	1630	763.6	1778	max K_{OC}, soil releases only

[a] Bolded values indicate which value was adjusted to test the sensitivity of the associated parameter (*i.e.*, half-life or K_{OC}).
[b] Mean water, soil, and sediment half-lives used, as in Run No. 1.

Note that these half-lives and release values were selected simply for this sensitivity analysis and are not proposed values for subsequent exposure and risk analyses. Otherwise, vinyl chloride properties were entered into EPI Suite™ as shown in Figure 3-1, and all other input variables to the LEV3EPI™ fugacity model were left at their default settings (*e.g.*, advection time). The results of the Tier II analysis are discussed in Section 3.2.2.

3.1.2 Evidence Integration for Fate and Transport Properties

As previously mentioned, EPA reviewed databases and previously conducted assessments to identify fate and transport properties to characterize the potential for vinyl chloride to persist in the environment or bioaccumulate, and to inform risk evaluation problem formulation. Through implementation of systematic review approaches as described in Sections 4 and 5 of the *Updated Search Strategies Used to Identify Potentially Relevant Discipline-Specific Information* (U.S. EPA, 2024b), EPA identified 1,682 data sources for the environmental fate characterization of vinyl chloride. Table 3-2 summarizes the information preliminarily identified for environmental fate and transport properties of vinyl chloride. These data were considered while identifying the major and minor compartments and pathways to inform problem formulation, and during preliminary media assessments for the purposes of this draft scope. Additionally, EPA integrated primary, peer-reviewed literature to help inform media assessments for which there was limited information available from databases and prior assessments. These primary sources were identified from early systematic review steps, though they have not yet been extracted and evaluated for quality following *Draft Systematic Review Protocol Supporting TSCA Risk Evaluations for Chemical Substances* (U.S. EPA, 2021) (also referred to as the "2021 Draft Systematic Review Protocol"). EPA will consider additional information and refine subsequent fate and transport analyses after the completion of the systematic review process during the development of the final scope and risk evaluation of vinyl chloride.

Table 3-2. Environmental Fate Properties of Vinyl Chloride

Property or Endpoint	Value[a]	Reference(s)
Direct photodegradation (air) *Section 3.3.2.1*	Does not absorb light at wavelengths >218 nm	ATSDR (2024)
	0.09 s^{-1} determined in static system, xenon lamp irradiation at 2.7 kW; 0.047 s^{-1} determined from flow experiments with 16-second residence time, xenon lamps at 3.7 kW	Reaxys (2023)
Direct photodegradation (water) *Section 3.3.2.2*	0% over 90 hours in water at 10 mg/L test substance concentration irradiated with >300 nm; absorption in water was <218 nm	OECD (2001)
Indirect photodegradation (air) *Section 3.3.2.1*	·OH-mediated: $t_{1/2}$ range of 1.27–2.71 days (n = 9; based on •OH rate constants of 3.95E–12 to 8.40E–12 cm^3/mole-sec and a 12-hour day with 1.5E06 ·OH/cm^3)	OECD (2001), ECHA (2023a), NLM (2023a), NIST (2023), ATSDR (2024)
	NO_3-mediated: $t_{1/2}$ range of 155 – 478 days (n = 6; based on NO_3 rate constants of 1.40E–16 to 4.30E–16 cm^3/mole-sec and a 12-hour day with 2.40E08 NO_3/cm^3)	ECHA (2023a), NIST (2023)
	O_3-mediated: $t_{1/2}$ range of 91.3 – 93.6 days (n = 2; based on O_3 rate constant of 2.45E–19 to 2.51E–19 cm^3/mole-sec and a 12-hour day with 7.0E11 O_3/cm^3)	ECHA (2023a), NLM (2023a)
Indirect photodegradation (water) *Section 3.3.2.2*	No decomposition over 20 hours at 10 mg/L test substance concentration in unfiltered Oconee River and Okefenokee Swamp water with 20 mg/l commercial humic acid	OECD (2001)
	80% over 3 hours at 10 mg/L test substance	OECD (2001)

Property or Endpoint	Value[a]	Reference(s)
	concentration, and H_2O_2 as a photosensitizer	
	Not readily degraded at 10 mg/L test substance concentration, with 1.0E–04 M methylene blue (singlet) and irradiation at 578 nm	OECD (2001)
	Rapid decomposition at 10 mg/L test substance concentration, with 10% vol. acetone and UV irradiation at 313 nm	OECD (2001)
Hydrolysis half-life (water) *Section 3.3.1*	$t_{1/2}$ > 9.91 years at 25 °C and pH 7 $t_{1/2}$ > 107 years at 10 °C and pH 7	NLM (2023a)
	$t_{1/2}$ > 1 year at both pH 4 and 6.1	OECD (2001)
	No degradation observed in water after 12 hours at 85 °C, at 20 mg/L test substance concentration; saturated with molecular oxygen	ATSDR (2024)
	<10 years at 25.5 °C and pH 4.3–9.4 (estimated)	OECD (2001), ATSDR (2024)
Abiotic reductive dehalogenation (water, soil) *Section 3.3.3*	<0.002 d^{-1} with zero-valent FeH_2, and 0.59 to 0.76 d^{-1} with zero-valent FeBH	Reaxys (2023)
	0.055, 0.323, 0.537, and 0.555 d^{-1} with Silawa loamy sand, montmorillonite, vermiculite and biotite, respectively, in the presence of Fe (II) at 22 °C and pH 7–7.2	Reaxys (2023)
	0.247, 0.355, and 0.358 d^{-1} with montmorillonite, vermiculite, and biotite, respectively, at 22°C and pH 7	Reaxys (2023)
	0.15 d^{-1} with Silawa loamy sand and dithionite at pH 7.2	Reaxys (2023)
	0.94 d^{-1} with green rust sulfate in Tris buffer at 22 °C and pH 8.1	Reaxys (2023)
Aerobic biodegradation (water) *Section 3.3.4.1*	21.5% over 5 days (CO_2 Evolution) at 0.05 mg/L test substance concentration, with municipal activated sludge inoculum, adaptation not specified	OECD (2001), ECHA (2023a)
	16% over 28 days (OECD 301D) at 2.04 mg/L test substance concentration, respectively; with sludge inoculum, adaptation not specified	NITE (2023), ECHA (2023a), NLM (2023a)
Aerobic biodegradation (sediment) *Section 3.3.4.2*	Complete dehalogenation within 28 days in a freshwater river sediment microcosm, following a 7-day lag period; non-adapted	Atashgahi et al. (2013)
Aerobic biodegradation (groundwater microcosms) *Section 3.3.4.4*	22–39% over 84 hours (mineralization) at approx. 1.13 mg/L test substance concentration in natural aquifer microcosm; some adaptation from chlorinated solvent and vinyl chloride contamination	Reaxys (2023), ATSDR (2024)

Property or Endpoint	Value[a]	Reference(s)
	>99% over 57 days, and >99% over 204 days at 330 µg/L test substance concentration, in groundwater/sediment batch microcosms; adaptation likely due to media exposure to vinyl chloride	NLM (2023a)
Aerobic biodegradation (soil) *Section 3.3.4.3*	>99% over 108 days (transformation) and 65% over 108 days (mineralization) at 1 mg/L test substance concentration in a natural shallow aquifer soil/groundwater microcosm, adaptation not specified	OECD (2001), ATSDR (2024) ECHA (2023a)
	1.456 µg/g soil/hour biodegradation in gas phase, incubated with soil from a landfill under methane oxidizing conditions, adaptation not specified	NLM (2023a)
Anaerobic biodegradation (water) *Section 3.3.4.1*	10% over 106 days following a 50-day lag at 2.6E–04 mg/L test substance concentration in groundwater containing H_2 and acetate, under methanogenic conditions; adaptation likely due to media exposure to vinyl chloride	Reaxys (2023)
	$t_{1/2}$ = 70 days at 0.4 mg/L test substance concentration, with groundwater bacteria inoculum, adaptation not specified	ECHA (2023a), NLM (2023a)
	$t_{1/2}$ = 110 days; study details not specified	NLM (2023a)
Anaerobic biodegradation (sediment) *Section 3.3.4.2*	5% to 44% over 37 days, and 8% to 100% over 37 days (mineralization) at 0.013 to 3.79 mg/L test substance concentration, in natural creek bed microcosm under methanogenic and Fe (III)-reducing conditions, respectively; some adaptation from former drum disposal area	Reaxys (2023), ATSDR (2024)
	50% over 25 days and 100% over 19 days with 0.02 and 0.1 mg/L dissolved oxygen, respectively, at 0.65 mg test substance; vinyl chloride-oxidizing culture inoculum in microcosm with media from contaminated site; adapted	ATSDR (2024)
	98% and 21% over 70 days in Naval Air Station, and Naval Weapons Industrial Reserve Plant sediment microcosms, respectively; under methanogenic conditions; some adaptation with preexposure of media to chlorinated solvents	ECHA (2023a)
	40% over 20 hours at 31.2 mg/L test substance concentration, in brackish sediment microcosm supplemented with methanol; adaptation not specified	Reaxys (2023)
	40% over 20 hours at 28.7 mg/L test substance concentration, in brackish	Reaxys (2023)

Property or Endpoint	Value[a]	Reference(s)
	sediment microcosm supplemented with H_2; adaptation not specified	
	Complete dehalogenation within 28 days in a freshwater river sediment microcosm, following a 7-day lag period; non-adapted	Atashgahi et al. (2013)
Anaerobic biodegradation (groundwater microcosms) *Section 3.3.4.4*	100% over 15 days in aquifer microcosm supplemented with methanol and C_2Cl_4; adaptation not specified	Reaxys (2023)
	100% over 14 weeks, and <20% over 14 weeks with and without supplemented electron donors,[c] respectively, in aquifer microcosm; some adaptation with media from vinyl chloride-contaminated site	Reaxys (2023)
	100% over >100 days at 39 mg/L test substance concentration in groundwater with sediment microcosm under Fe- and SO_4^--reducing conditions; some adaptation with media from contaminated site	Reaxys (2023)
	15–34% over 84 hours, and 2.8–4.6% over 84 hours (mineralization) at approx. 1.13 mg/L test substance concentration, in natural aquifer microcosm, amended with Fe(III) and unamended, respectively; some adaptation from media exposure to chlorinated solvents and vinyl chloride	Reaxys (2023), ATSDR (2024)
Anaerobic biodegradation (soil) *Section 3.3.4.3*	$t_{1/2}$ of 4 weeks at 0.4 mg/L test substance concentration, in sand/water microcosm; adaptation not specified	ECHA (2023a), NLM (2023a)
Bioconcentration factor (BCF) (L/kg wet weight [ww]) *Section 3.6*	BCF <10 in Golden Ide (*Leuciscus idus* melanotus)	OECD (2001), ATSDR (2024), NLM (2023a), ECHA (2023a)
	BCF = 40 in green algae (*Chlorella fusca*)	OECD (2001), ATSDR (2024), NLM (2023a), ECHA (2023a)
	Upper Trophic Level: 3.168 Middle Trophic Level: 2.482 Lower Trophic Level: 2.310	EPI Suite™ (BCFBAF, Arnot-Gobas method)[b]
Bioaccumulation factor (BAF) (L/kg ww, unless noted) *Section 3.6*	Upper Trophic Level: 3.168 Middle Trophic Level: 2.482 Lower Trophic Level: 2.310	EPI Suite™ (BCFBAF, Arnot-Gobas method)[b]
Organic carbon:water partition coefficient (log K_{OC}) (soil) *Section 3.2.1*	2.38–2.95 in seven natural clayey till soil samples	ATSDR (2024)
	1.75	OECD (2001), NLM (2023a)

Property or Endpoint	Value[a]	Reference(s)
Removal in wastewater treatment *Section 3.5.3*	Total removal: 91.54% Losses to stripping: ~89%	EPI Suite™ (STPWIN, with default biodegradation $t_{1/2}$s = 10,000 h)[b]

[a] Measured unless otherwise noted
[b] Information was estimated using EPI Suite™ (U.S. EPA, 2017).
[c] H_2, formate, acetate, pyruvate, lactate, fumarate, glycerol, glucose, molasses, or whey.

3.2 Partitioning, and Major and Minor Pathways

3.2.1 Tier I Analysis

Environmental transport and partitioning consist of processes such as volatilization, advection, dispersion, diffusion, association with dissolved organic matter, and sorption to solids. These processes, in turn, are controlled by physical and chemical interactions between vinyl chloride and the surrounding media (*e.g.*, air, water, soil, sediments, etc.). Vinyl chloride released to the environment is subject to these processes, though some processes are more likely or prevalent than others based on its physical and chemical characteristics.

To be able to understand and predict the behaviors and effects of vinyl chloride in the environment, the first step is identifying partitioning values (Table 3-3), which can provide insight into how vinyl chloride may favor one media over another.

Table 3-3. Partitioning Values for Vinyl Chloride

Partition Coefficient	Value[a]	Log Value	Source(s)	Predominant Phase[d]
Octanol:Water (K_{OW})	24.0	1.38	Rumble (2023), ATSDR (2024), ECHA (2023c)	Octanol/Organic Phase
Organic Carbon:Water (K_{OC})	382	2.58 (range 1.75–2.95)	Average of values (n = 8) reported in OECD (2001), NLM (2023a), ATSDR (2024)	Organic Carbon
Octanol:Air (K_{OA})	21.1	1.324	EPI Suite™ (KOAWIN)[b]	Organic Carbon
Air:Water (K_{AW})	1.14	0.056	Calculated[c] using Henry's Law constant (HLC) reported in PhysProp (2023)	Air

[a] Measured unless otherwise noted
[b] Information was estimated using EPI Suite™ (U.S. EPA, 2017)
[c] Calculated using the relationship: $HLC = R * T * K_{AW}$, where R is the universal gas constant 8.206×10^{-5} atm·m^3/mol·K
[d] Predominant phases displayed assume an evaluative environment where the relevant media exist in a 1:1 ratio

The magnitude of the above-listed partitioning coefficients suggest that vinyl chloride will exist primarily in air and water in the environment. Vinyl chloride has a vapor pressure of 2,550 mmHg at 20 °C (ECHA, 2023a) indicating that vinyl chloride will exist predominantly as a free gas in the atmosphere, and dry deposition is unlikely to be an important process. This is consistent with the estimated octanol:air partition coefficient of 25.4 (U.S. EPA, 2017).

With a HLC of 0.0278 atm·m^3/mol at 24.8 °C (PhysProp, 2023), vinyl chloride is also expected to be volatile from surface water. The calculated air:water partition coefficient is very close to unity (1.14; Table 3-3), suggesting that at equilibrium, vinyl chloride will partition approximately equally between air and water media, with a slight preference for air. However, because the partial pressure of vinyl chloride above natural bodies of water is likely to exist below its vapor pressure, volatilization from surface water is expected to be a rapid and dominant pathway.

While volatile, vinyl chloride also has considerable water solubility (9,150 mg/L at 20.5 °C (ECHA, 2023a; Reaxys, 2023)) consistent with its polarity and small molecular size. Dissolved salts in water can also impact the degree to which vinyl chloride remains in aqueous phase: salts of iron, silver, copper, platinum, iridium, and mercury have been shown to form complexes with vinyl chloride, slowing competing volatilization processes (ATSDR, 2024; IPCS, 1999). Intermediate sorption to organics present in sediments and suspended and dissolved solids present in water is expected given the range of log K_{OC} values identified during screening (Table 3-2), discussed further below.

Two sources were identified reporting log K_{OC} values for vinyl chloride. The first reported a log K_{OC} value of 1.75, but without additional detail on materials or methods (NLM, 2023a; OECD, 2001). The second is an empirical study following OECD 106 guidelines that investigated seven low-OC, natural clayey till soils from Denmark, reporting log K_{OC} values ranging from 2.38 to 2.95 (mean 2.70) (ATSDR, 2024). The authors highlighted that in addition to the organic carbon content of the soil, the clay content and specific surface area of the soil particles influenced the adsorption coefficient values obtained for vinyl chloride, especially on low-OC soils (Lu et al., 2011). Vinyl chloride's solubility along with its moderate tendency to sorb to organics present in solids suggest that vinyl chloride that occurs in soil will exhibit some mobility and may be transported through the vadose zone to groundwater.

3.2.2 Tier II Analysis

Table 3-4. EPI Suite^{TM} Level III Fugacity Modeling Results for Vinyl Chloride

Release Source	Run No.	Percent (%) Mass Distribution by Media				Run Notes
		Air	Water	Soil	Sediment	
TRI RELEASES	1	99.8	<1	<1	<1	min K_{OC}; mean water, soil, and sediment $t_{1/2}$
	2	99.5	<1	<1	<1	max K_{OC}; mean water, soil, and sediment $t_{1/2}$
	3	99.8	<1	<1	<1	min K_{OC}, max water $t_{1/2}$
	4	99.8	<1	<1	<1	min K_{OC}, min water $t_{1/2}$
	5	99.8	<1	<1	<1	min K_{OC}, max soil $t_{1/2}$
	6	99.8	<1	<1	<1	min K_{OC}, min soil $t_{1/2}$
	7	99.8	<1	<1	<1	min K_{OC}, max sediment $t_{1/2}$
	8	99.8	<1	<1	<1	min K_{OC}, min sediment $t_{1/2}$
"GENERIC" RELEASES[a]	9	27.2	68.3	4.33	<1	min K_{OC}, equal releases
	10	18.5	49	31.4	1.06	max K_{OC}, equal releases
	11	8.78	90.9	<1	<1	min K_{OC}, water releases only
	12	8.63	89.4	<1	1.93	max K_{OC}, water releases only

Release Source	Run No.	Percent (%) Mass Distribution by Media				Run Notes
		Air	Water	Soil	Sediment	
	13	69.4	1.08	29.5	<1	min K_{OC}, soil releases only
	14	16.8	<1	83	<1	max K_{OC}, soil releases only

[a] Mean water, soil, and sediment half-lives used, as in Run No. 1.

Table 3-4 presents the mass percentage distribution of vinyl chloride by media for each of the 14 LEV3EPI^{TM} model runs. The first set using TRI release data (see Section 3.1.1 for additional information on TRI data) as the emission rates (runs one through eight) indicate that when the vast majority of vinyl chloride is released to air, the vast majority (>99.5%) will also remain in the air compartment. This result was not impacted by varying vinyl chloride's K_{OC} value or half-lives in water, soil, or sediment. From the generic release scenarios (runs nine through 14), it is apparent that the affinity of vinyl chloride to soil (governed by its log K_{OC}) will greatly influence the fraction that remains in soil vs. the fraction that volatilizes from soil: when emissions were exclusively to the soil compartment and the minimum K_{OC} value was used, about 69 percent of vinyl chloride was transported to air while about 30 percent remained in soil. Conversely, when run with the maximum K_{OC}, only about 17 percent volatilized to air, with 83 percent remaining in the soil. A similar trend is apparent in the soil fractions from runs nine and ten under equal releases. Note that the vinyl chloride fractions estimated to remain in soil as modeled with LEV3EPI^{TM} (steady state, with constant releases) may be greater than those at equilibrium after a single, pulse release to soil. This highlights the competition between soil-to-air volatilization and sorption to soil that may vary depending on site-specific soil properties and thus sorption affinity.

When vinyl chloride was released exclusively to the water compartment, approximately 91 percent of the chemical remained in water, with about nine percent volatilizing to air. These ratios were largely unaffected by the K_{OC} value used. The graphical results of the LEV3EPI^{TM} model runs are presented in Figure 3-2.

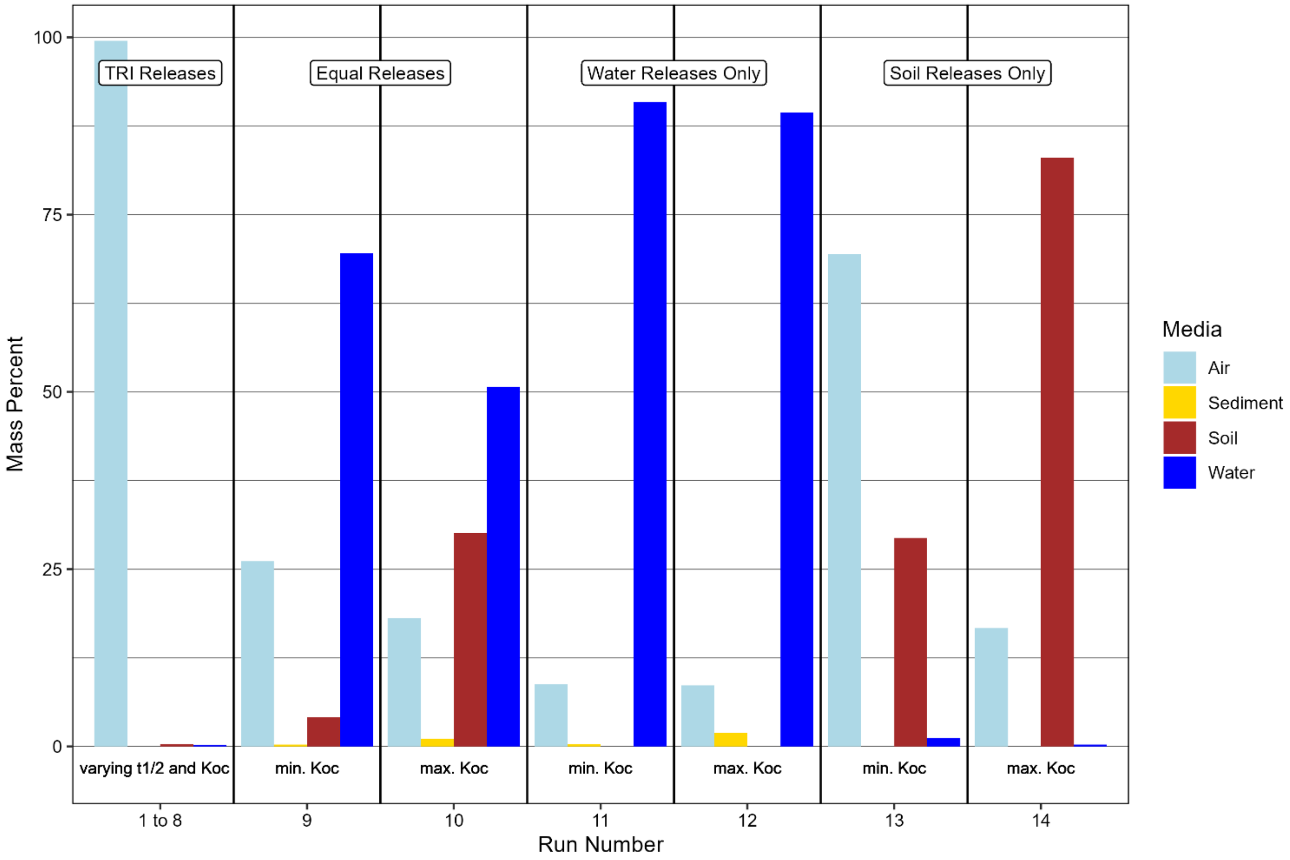


Figure 3-2. EPI Suite^{TM} Level III Fugacity Modeling Graphical Result for Vinyl Chloride

From the results of these partitioning and fugacity exercises, it is evident that the air compartment and associated transformation pathways will be major pathways in the assessment of vinyl chloride. As TRI data provide the best available information on the distribution of vinyl chloride releases among the environmental media, the fugacity model runs using TRI releases increase confidence that vinyl chloride will primarily be present in the atmosphere. To contrast, the fugacity model runs using generic releases are not representative of expected media releases but provide information on vinyl chloride's intermedia transport and partitioning dynamics, as discussed further below.

Though there are proportionally very low reported releases to water, by virtue of its partitioning behavior and water solubility, vinyl chloride that is released to water (*e.g.*, from spills and leaks) will tend to remain in water, especially in instances with limited air/water interface. Because of this, water should be considered as a major compartment in such localized and/or continuous release instances. Similarly, results of the fugacity modeling indicate that in instances of vinyl chloride release to soil, a large proportion will remain in soil with the remainder volatilizing to the air compartment. It should be noted that vinyl chloride is expected to migrate rapidly to groundwater from soil, a pathway that is not explicitly described in the LEV3EPI^{TM} model. Nonetheless, in areas of continuous release to soil—especially where the soil properties favor adsorption—a fraction of vinyl chloride may remain in the soil. The sediment compartment may be considered as a minor compartment, as it consistently yielded negligible proportions of vinyl chloride across all model runs.

3.3 Transformation Processes

3.3.1 Hydrolysis

Hydrolysis is a form of a chemical reaction where water, often in combination with light energy or heat, breaks down one or more chemical bonds in a chemical substance. Hydrolysis half-life indicates the rate at which a chemical will react with water. Predicting hydrolysis rates can help to estimate how long the chemical and/or its hydrolysis byproducts will remain after being released to the environment.

The identified hydrolysis data indicate that vinyl chloride undergoes negligible hydrolysis in aqueous environments. One study reported hydrolysis half-lives of greater than one year at pH 4 and 6.1, greater than 9.91 years at 25 °C and pH 7, and greater than 107 years at 10 °C and pH 7 (NLM, 2023a; OECD, 2001). Another study observed no hydrolysis of vinyl chloride over 12 hours at 85 °C under saturated molecular oxygen conditions (ATSDR, 2024). Because other intermedia transport (*i.e.*, volatilization) and aquatic transformation pathways occur over much shorter timescales, hydrolysis is not expected to be an important transformation pathway for vinyl chloride.

3.3.2 Photolysis

Photolysis is a chemical reaction in which chemical molecules are broken down via the energy in light. There are two forms of photolysis: direct and indirect. Direct photolysis occurs when a chemical substance is able to absorb direct sunlight at wavelengths within the atmospheric window (*i.e.*, wavelengths greater than 290 nm that are able to pass through earth's atmosphere). Indirect photolysis occurs in the presence of photosensitizers (*e.g.*, ozone (O_3), nitrate (NO_3), and hydroxyl radicals (·OH), etc.) under visible light.

3.3.2.1 Atmosphere

Vinyl chloride is not expected to undergo direct photolysis in the environment, as it does not absorb wavelengths above 218 nm (ATSDR, 2024). It was demonstrated that vinyl chloride can degrade rapidly under controlled irradiation conditions in laboratory settings: vinyl chloride was degraded in stainless steel reactors at a rate of 0.09 s^{-1} under static conditions irradiated with xenon lamps at 2.7 kW (Reaxys, 2023). The same study measured a direct photolysis rate of 0.047 s^{-1} under flow conditions with a 16-second reactor residence time and 3.7 kW xenon lamps (Reaxys, 2023). The authors noted that the output efficiency of the xenon lamps was 18.6 percent of input wavelength distribution less than or equal to 300 nm (Reaxys, 2023). While these data demonstrate that vinyl chloride may undergo direct photolysis under controlled laboratory conditions, these rates may not be representative of typical conditions in the atmosphere.

Several studies reported indirect photolysis rates for vinyl chloride by ozone (O_3), nitrate (NO_3), and hydroxyl radicals (·OH). Nine studies reported ·OH-mediated degradation rates of 3.95×10^{-12} to 8.40×10^{-12} cm^3/mole-sec (ATSDR, 2024; ECHA, 2023a; NIST, 2023; NLM, 2023a; OECD, 2001). Assuming a 12-hour day and an atmospheric ·OH concentration of 1.5×10^{6} ·OH/cm^3, the identified degradation rates translate to a half-life range of 1.27 to 2.71 days, with a mean of 1.84 days. Because the ·OH-mediated half-lives are the shortest of all those identified (see Table 3-2), the ozone- and nitrate-mediated experiments will not be discussed further. Based on the ·OH-mediated photolysis half-lives, vinyl chloride may have high persistence potential in the atmosphere, defined as an atmospheric half-life greater than 2 days (64 FR 692; January 5, 1999).

3.3.2.2 Surface Water

Direct photolysis of vinyl chloride is expected to be negligible. One study reported no decomposition of 10 mg/L of vinyl chloride after 90 hours of irradiation at wavelengths greater than 300 nm. The same study reported a wavelength absorption range of below 218 nm (OECD, 2001).

Identified data for indirect photolysis of vinyl chloride in aqueous systems suggest that rapid degradation can occur in the presence of certain photosensitizers and wavelengths, though vinyl chloride may also remain stable. An indirect, aqueous photolysis degradation rate of 80 percent over 3 hours was observed with 10 mg/L of vinyl chloride in the presence of H_2O_2 (OECD, 2001). A second study noted rapid decomposition (no rate information provided) of vinyl chloride in solution with 10 percent acetone by volume and 313-nm UV irradiation (OECD, 2001). To contrast, no decomposition was observed in Oconee River and Okefenokee Swamp (Georgia, United States) water containing 20 mg/L of commercial humic acid, nor was it observed in the presence of methylene blue in aqueous solution irradiated at 578 nm (OECD, 2001). Though there exists some evidence for rapid degradation via indirect photolysis under certain aqueous conditions, vinyl chloride's volatility from water (HLC 0.0278 $atm{\cdot}m^3/mol$ (PhysProp, 2023)) will likely outcompete this transformation route, thus indirect photolysis is unlikely to be an important removal pathway for vinyl chloride from water.

3.3.3 Abiotic Dehalogenation

In addition to hydrolysis, vinyl chloride may be degraded via reductive abiotic processes, namely reductive dechlorination. Reductive dechlorination (also hydrogenolysis) is a process that reduces a chlorinated compound via the substitution of a chlorine atom with a hydrogen atom, a common degradation pathway for chlorinated ethenes under anaerobic conditions (Tobiszewski and Namieśnik, 2012).

The degree of susceptibility of vinyl chloride to abiotic dehalogenation relies on the minerality of the anaerobic system: of those determined only with minerals characteristic of soil and aquifer systems, rates of 0.055 to 0.15 d^{-1}, 0.247 to 0.323 d^{-1}, 0.355 to 0.537 d^{-1}, and 0.358 to 0.555 d^{-1} were determined with Silawa loamy sand, montmorillonite, vermiculite, and biotite, respectively (Reaxys, 2023). Assuming first order kinetics, these equate to half-lives ranging from 1.25 to 12.6 days, suggesting that abiotic dehalogenation may serve as an important degradation process in deep, anaerobic soil conditions that may exist in natural aquifers. However, it has been noted that the extent of dehalogenation relies on the concentration of reductants (*e.g.*, Fe(II), dithionite) present in the system (Lee and Batchelor, 2004).

3.3.4 Biodegradation

Biodegradation occurs when an organic material is broken down by microorganisms. Many of the biodegradation data identified to date—namely microcosm studies—were collected using media (*i.e.*, sediment, soil, water) and/or microbial inoculums originating from sites with histories of exposure to vinyl chloride and often other chlorinated solvents (ATSDR, 2024; NLM, 2023a; Reaxys, 2023). For the purposes of this draft scope, data collected with pre-exposed media or microbes are assumed to have adapted to growth in the presence of vinyl chloride and/or similar solvents. While results from biodegradation studies employing adapted media and microbes may not be readily applied to the general, uncontaminated environment, they may serve to inform scenarios in which localized or predictable vinyl chloride release(s) may occur (*e.g.*, spills or leaks near manufacturing sites).

3.3.4.1 Surface Water

Two aqueous aerobic biodegradation studies were identified for vinyl chloride. The first study followed OECD 301D test guidelines and reported a degradation rate of 16 percent over 28 days at an initial vinyl chloride concentration of 2.04 mg/L (ECHA, 2023a; NITE, 2023; NLM, 2023a). The additional study a reported mineralization rate of 21.5 percent over five days (ECHA, 2023a; OECD, 2001). Additional inoculum details may be found in Table 3-2.

Though not explicitly representative of anaerobic surface water, three studies were also identified reporting biodegradation rates of vinyl chloride under various anaerobic aqueous conditions. One resource reported a half-life of 110 days though without any additional study details (NLM, 2023a). The second source, cited by both ECHA (2023a) and NLM (2023a), reported a half-life of 70 days in water containing 0.4 mg/L of vinyl chloride and inoculated with groundwater bacteria. The third study reported 10 percent degradation over 106 days following a 50-day lag period in groundwater containing H_2, acetate, and 2.6×10^{-4} mg/L of vinyl chloride (Reaxys, 2023). Taken together, these studies indicate that vinyl chloride is considered not readily biodegradable and will likely undergo slow biodegradation in surface water under both aerobic and anaerobic conditions.

3.3.4.2 Sediment

In sediments, vinyl chloride may be transformed via different routes of microbial biodegradation, depending on oxygen availability. In the suboxic layer below surface sediments, vinyl chloride and other chlorinated ethenes (*e.g.*, PCE, TCE) may serve as terminal electron acceptors for both facultative and obligate organohalide-respiring heterotrophic bacteria. The extent and rate of anaerobic chlorinated ethene reduction rely on the presence, characteristics, and concentrations of electron donors (*e.g.*, dissolved organic matter, molecular hydrogen) and other competing and complementary electron acceptors (*e.g.*, nitrate, sulfate, iron), as the microbial degradation of chlorinated ethenes in sediments intersects common biogeochemical processes (Weatherill et al., 2018). In surface sediments, aerobic respiration may occur if overlying water is able to bring dissolved oxygen and organic matter into the sediment by advection and diffusion to the interstitial pore water. This creates a sediment layer in which oxidation of vinyl chloride may occur, sometimes via co-metabolic or mineralization routes (Weatherill et al., 2018; Atashgahi et al., 2013).

From the data identified to date, the anaerobic biodegradation rate for vinyl chloride in sediments can vary widely with redox conditions. One study observed the biodegradation of 0.013 to 3.79 mg/L of vinyl chloride in a creek sediment bed microcosm to range from 5 to 44 percent over 37 days under methanogenic conditions, and 8 to 100 percent over 37 days under Fe(III)-reducing conditions (ATSDR, 2024; Reaxys, 2023). Assuming first-order kinetics, these rates equate to $t_{1/2}$'s of 500, 44, 308, and 2.2 days, respectively (mean 213.5 days). ECHA (2023a) cited a study that reported 98 and 21 percent degradation under methanogenic conditions over 70 days in microcosms containing sediments collected from the Naval Air Station (Cecil Field) and Naval Weapons Industrial Reserve Plant (Dallas, TX), respectively. Preexposure of the sediments to chlorinated solvents (dichloroethylene [DCE], TCE and vinyl chloride) from contaminated groundwater was noted by the authors, suggesting possible adaptation (ECHA, 2023a). Another pair of anaerobic biodegradation studies demonstrated rapid vinyl chloride degradation rates (both 40 percent over 20 hours) in brackish sediment microcosms when supplemented with methanol and H_2 and starting test concentrations of 31.2 and 28.7 mg/L, respectively (Reaxys, 2023). In an autochthonous, unamended freshwater river sediment microcosm, vinyl chloride was rapidly degraded under both anaerobic and aerobic conditions across three sequential additions of vinyl chloride: after a seven-day lag period, complete dehalogenation was observed in the anaerobic microcosms within 28 days after the first vinyl chloride spike. This rate increased to complete dehalogenation within 14 days after the third spike, indicating the ability for the system to adapt to vinyl chloride as a substrate. The same study noted similar degradation kinetics under aerobic conditions (Atashgahi et al., 2013). Given this preliminarily identified information, biodegradation rates of vinyl chloride in sediments are expected to vary widely depending on the redox conditions, electron donor availability, and previous exposure of the microbial community to vinyl chloride.

3.3.4.3 Soil

Similar to sediments, soils can contain gradients of environmental variables (*i.e.*, oxygen, minerality, organic co-substrates, water saturation) that dictate rates, routes, and extent of biodegradation. Because of this, the rate of vinyl chloride biodegradation in soil can vary dramatically based on the test system characteristics. In an aerobic microcosm containing natural soil and groundwater from a shallow aquifer, vinyl chloride was degraded greater than 99 percent (transformation) and 65 percent (mineralization) within 108 days (ATSDR, 2024; ECHA, 2023a; OECD, 2001). A degradation rate of 1.456 µg/g-soil-hour was observed for vinyl chloride gas incubated under methane oxidizing conditions with soil cover from a landfill in Denmark (NLM, 2023a).

In an anaerobic sand/water microcosm study, vinyl chloride was reported to have a half-life of 4 weeks when tested at a 0.4 mg/L test concentration (ECHA, 2023a; NLM, 2023a). Based on soil biodegradation rates identified to date, vinyl chloride is expected to biodegrade slowly in soils, therefore, biodegradation is not expected to be an important mechanism for vinyl chloride removal from soil.

3.3.4.4 Groundwater

Subterranean environments where groundwater exists contain gradients of environmental variables (*i.e.*, oxygen, minerality, organic co-substrates) that dictate rates, routes, and extent of biodegradation. While it is possible for aerobic conditions to exist in groundwaters, for instance, where exchanges with oxygenated surface waters occur, groundwater environments are often anaerobic in nature. Because of the many influencing factors, the rate of vinyl chloride biodegradation in groundwater can vary dramatically based on the test system characteristics. Two data sources were identified reporting the aerobic biodegradation of vinyl chloride in aquifer microcosms containing groundwater and sediments. The first study reported 22 to 39 percent mineralization of vinyl chloride over 84 hours (3.5 days) starting from an initial concentration of 1.13 mg/L (ATSDR, 2024; Reaxys, 2023). The second study reported greater than 99 percent vinyl chloride degradation over both 57 and 204 days in groundwater/sediment batch microcosms using media collected from areas with a history of vinyl chloride contamination (NLM, 2023a).

Four sources were identified reporting the anaerobic biodegradation of vinyl chloride in aquifer microcosms. Three of these reported using media from vinyl chloride-contaminated sites: the first reported mineralization rates of 2.8 to 4.6 percent over 84 hours in a microcosm containing natural aquifer materials, and 15 to 34 percent over 84 hours in aquifer microcosms amended with Fe(III) (ATSDR, 2024; Reaxys, 2023). The second study observed complete vinyl chloride biodegradation after greater than 100 days in a sediment/groundwater microcosm under iron and sulfate-reducing conditions (Reaxys, 2023). The third study noted less than 20 percent vinyl chloride degradation over 14 weeks in an aquifer microcosm, though this proportion increased to 100 percent in microcosms supplemented with additional electron donors (Reaxys, 2023). The final anaerobic groundwater degradation rate identified was 100 percent vinyl chloride degradation over 15 days in an aquifer microcosm supplemented with methanol and PCE (Reaxys, 2023).

From the evidence gathered to date on the biodegradation of vinyl chloride in groundwater media, it is expected that vinyl chloride may degrade slowly to rapidly in groundwater depending on the chemistry of the groundwater media. Such influencing factors include the presence or absence of additional organic electron donors, the minerality of the system, the concentration and adaptability of the microbial population, and the redox conditions.

3.3.4.5 Vinyl Chloride as a Transformation Product

Vinyl chloride has been reported as a transformation product of other chlorinated organic compounds, and therefore some instances of vinyl chloride in the environment may be due to the uses of those parent chemicals rather than direct uses of vinyl chloride. PCE and TCE are two of the most commonly reported precursors of vinyl chloride: in anaerobic environments, more highly-chlorinated ethylene solvents may undergo sequential reductive dehalogenation following the pathway:

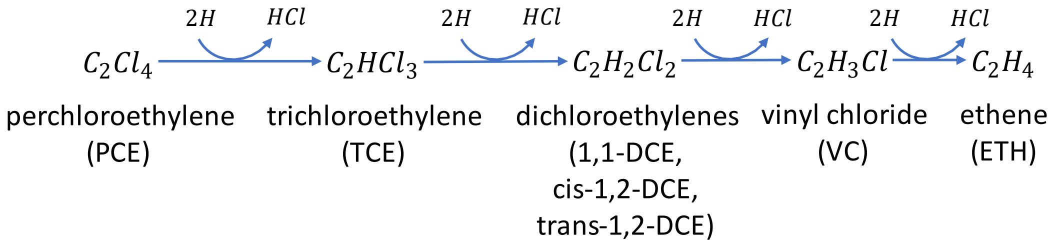


Figure 3-3. Reductive Dechlorination Pathway via Biodegradation in Anaerobic Environments

Adapted from (Eklund et al., 2022; Freedman and Gossett, 1989; Molton et al., 1987).

The relative rates of dechlorination proceed such that the half-lives of PCE and TCE are much shorter than those of 1,1- and 1,2-DCEs and vinyl chloride. Wood (1985) reported half-lives of 34, 43, and 53 days for PCE, TCE, and 1,1-DCE, respectively, while there was no detectable reduction of 1,2-DCEs and vinyl chloride. Historically, this has led to accumulation and presence of DCEs and vinyl chloride in groundwater where only PCE and/or TCE were known to have been released (Lee et al., 2015; Hunkeler et al., 2011; Milde et al., 1988). This is consistent with observations that the vinyl chloride-to-ethene reduction is the rate limiting step during complete dechlorination in controlled systems (Freedman and Gossett, 1989). The composition of microbial communities and redox conditions also dictate the kinetics and extent to which the degradation pathway illustrated in Figure 3-3 may proceed (Lee et al., 2015; Hunkeler et al., 2011). Dechlorination of more highly-chlorinated ethylenes yielding vinyl chloride has also been reported as an important source of vinyl chloride in landfills (Molton et al., 1987).

3.4 Media Assessments

As discussed in Section 3.1, EPA reviewed databases and previously conducted assessments to gather data informing the preliminary fate and transport presented in this draft scope. While EPA does not expect high-level conclusions on the fate and transport of vinyl chloride to change significantly, the fate assessment will be further developed as the workflow outlined in the 2021 Draft Systematic Review Protocol is completed through the final scoping and risk evaluation processes. Therefore, the following media assessments are not final, but rather presented to inform problem formulation and analysis plans for subsequent risk evaluation development.

3.4.1 Air and Atmosphere

3.4.1.1 Outdoor Air

As presented in Section 2.3.1 of the *Draft Scope of the Risk Evaluation for Vinyl Chloride* (U.S. EPA, 2025), greater than 98 percent of the reported vinyl chloride releases are to air. Additionally, it is expected that vinyl chloride released to surface water and wastewater treatment plants (WWTPs) will rapidly volatilize to the air compartment. Similarly, vinyl chloride present in the top layers of soils and landfills is expected to volatilize rapidly. Vinyl chloride has a vapor density of 2.21 (relative to air = 1; see

Table 2-1), therefore vinyl chloride vapor may settle in stagnant air (*i.e.*, without mixing or wind).

Vinyl chloride reacts with hydroxyl radicals (·OH) with transformation rates reported between 3.95×10^{-12} and 8.40×10^{-12} cm^3/mole-sec (ATSDR, 2024; ECHA, 2023a; NIST, 2023; NLM, 2023a; OECD, 2001). Assuming a ·OH concentration of 1.5×10^6 ·OH/cm^3 and 12 hours of sunlight, the half-life of vinyl chloride may range from 1.27 to 2.71 days, with a mean of 1.84 days.

Vinyl chloride is expected to have a low tendency to associate with particulates in the atmosphere and will predominately be in the gaseous phase (see Section 3.2.1). Because of this, the majority of vinyl chloride present in the atmosphere is expected to be subject to indirect photolysis with low-to-moderate potential for long-range transport (LRTP).[1] However, as air is a major compartment for vinyl chloride, these conclusions will be confirmed and revised as appropriate during final scoping and risk evaluation phases with the completion of systematic review and the final fate assessment.

3.4.1.2 Indoor Air and Dust

Vinyl chloride may be present in indoor air due to volatilization from contaminated municipal water or well water (see Section 3.5.2), volatilization from consumer products containing vinyl chloride, and via vapor intrusion in areas with contaminated groundwater and soils (Eklund et al., 2022). Vapor intrusion occurs when groundwater or soil is contaminated by a volatile chemical that then diffuses through subsurface soil, eventually migrating into buildings above. Buildings with appropriately maintained vapor barriers separating bare soil and the lowest level are expected to have less susceptibility to vapor intrusion, though the characteristics of the barrier and the chemical of concern will dictate potential for barrier permeation. Ecklund et al. (2022) performed a series of four field groundwater/soil monitoring case studies representing various aquifer depths and soil types; they demonstrated that vinyl chloride in contaminated groundwater will evaporate yielding deep soil vapor concentrations ranging from not detected (ND; site LODs ranging from 0.013 to 3.9 µg/m^3) up to 47,000 µg/m^3, and will diffuse upward through the pore space in soil. However, surface soil vapor concentrations of vinyl chloride were significantly lower than the deep soil levels at all four sites, and all indoor air concentrations were below detection limits. The authors expect that the removal of vinyl chloride in the vadose zones was largely due to aerobic biodegradation that was faster than the rate of upward diffusion (Eklund et al., 2022). Vinyl chloride occurrence in groundwater and soil resulting from the conditions of use (COUs) considered in this draft scope is also expected to be negligible (see Figure 2 in *Draft Scope of the Risk Evaluation for Vinyl Chloride*). Therefore, vapor intrusion is not expected to be an important exposure pathway for vinyl chloride under TSCA.

In indoor air, vinyl chloride in the gas phase is expected to be more persistent as compared to outdoor environments. Indoor environments have fewer physical transport drivers (*e.g.*, advection by wind and atmospheric flows) as well as less sunlight and subsequently lower concentrations of hydroxyl radicals. Therefore, vinyl chloride transformation rates are expected to be slow in indoor air. Since vinyl chloride is not likely to sorb to particulates in air (see Section 3.2.1), partitioning to dust is not expected to be an important pathway.

3.4.2 Aquatic Environments

Vinyl chloride may enter aquatic environments from direct releases from industrial processes (including leaks and spills) or transport from groundwater through sediment layers in aquifer-fed bodies of water (Weatherill et al., 2018; Atashgahi et al., 2013). As discussed in Sections 3.1.1 and 3.2.2, TRI reports small fractions of releases to surface waters. Ambient monitoring data retrieved from the Water Quality Portal (WQP) from samples collected between 2017 and 2021 showed zero of the 1,358 surface water

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[1] Beyer et al., (2000) classifies a characteristic travel distance (CTD) of less than 600 km as low, a CTD between 600 and 1,100 km as moderate, and a CTD above 1,100 km as high chemical LRTP.

samples collected contained quantifiable vinyl chloride concentrations. In surface water samples collected in 2022 and 2023, one of the 69 samples contained detectable vinyl chloride at a concentration of 0.5 ppb. Similarly, one sample of the 306 sediment samples collected between 2011 and 2021 contained quantifiable vinyl chloride (1,300 ppb) (ATSDR, 2024).

3.4.2.1 Surface Water

Vinyl chloride may enter surface waters through anticipated releases, migration of landfill leachate, and releases from spills and leaks. As described above, vinyl chloride is not expected to undergo wet or dry deposition (see Section 3.4.1.1). Vinyl chloride may also form in anaerobic media from the reductive dehalogenation of more highly-chlorinated ethylene contaminants (*e.g.*, PCE, TCE; see Section 3.3.4.5).

Although vinyl chloride present in surface water is expected to volatilize appreciably, some fractions may remain dissolved in the aqueous phase and to a lesser extent adsorbed to organics found in suspended solids, as indicated by the log K_{OC} values presented in Table 3-2. Of the small amount of vinyl chloride that may remain in aqueous phase in surface water is expected to persist; because hydrolysis of vinyl chloride is unlikely (see Section 3.3.1), transformation of vinyl chloride in water is expected to be primarily mediated by biodegradation processes.

Aerobic ready biodegradation studies identified to date indicate that vinyl chloride is not readily biodegradable (see Section 3.3.4.1). Anaerobic biodegradation rates range from 10 percent over 106 days in water under methanogenic conditions following a 50-day lag, to 50 percent over 28 days in a sand/water microcosm (ECHA, 2023a; NLM, 2023a; Reaxys, 2023). An aerobic degradation rate of greater than 99 percent over 108 days (transformation) was reported for an aerobic soil/groundwater microcosm (ATSDR, 2024; ECHA, 2023a; OECD, 2001). The degree of vinyl chloride biodegradation is therefore expected to vary with microbial community, the level of adaptation of the present microbial community, and environmental conditions. Given the range of empirical aerobic biodegradation half-lives, vinyl chloride is expected to have moderate to high persistence (defined as $t_{1/2}$ 60–179 days, and greater than or equal to 180 days, respectively) in the surface water compartment under environmentally relevant conditions. Despite not being readily biodegradable, vinyl chloride is not widely or frequently detected in aquatic environments, likely due to minimal releases to water and its tendency to volatilize rapidly.

3.4.2.2 Sediments

While the majority of vinyl chloride that enters surface water bodies is likely to volatilize, some may remain in the water column and become transported to sediments via diffusion and advection or, to a lesser extent, associated with particulate organic matter. Vinyl chloride may also enter sediments and subsequently surface water bodies via diffusion from contaminated groundwater at aquifer/surface water interfaces (Weatherill et al., 2018).

No empirical data on vinyl chloride adsorption to sediment were identified. Based on empirical soil log K_{OC} values, however, vinyl chloride in the water column is not expected to partition significantly to organics in sediment. Vinyl chloride may be transported by diffusion and advection processes to sediment pore water. Given the range of anaerobic biodegradation rates identified in aqueous microcosms containing surface water sediment media (see Section 3.3.4.2), vinyl chloride is expected to persist with a mean half-life of 213.5 days in natural, non-adapted creek bed sediment (ATSDR, 2024; Reaxys, 2023). Other anaerobic sediment and aquifer sediment/groundwater microcosm studies have reported much faster degradation rates, though many of these used media from vinyl chloride-contaminated areas which may have increased degradation rates via adaptation (see Table 3-2). However, as indicated by fugacity modeling (see Section 3.2.2) and identified monitoring data (see

Section 3.4.2), vinyl chloride is not likely to be present in sediments.

3.4.3 Terrestrial Environments

Vinyl chloride may enter terrestrial environments via the disposal of industrial processing wastes, the degradation of more highly-chlorinated ethylenes (see Section 3.3.4.5), and incidental spills and leaks. Because the majority of reported releases are to air (see Section 3.2.2), and releases to soil media are expected to volatilize rapidly, terrestrial environments and processes are not expected to be significant to the evaluation of vinyl chloride. However, terrestrial fate of vinyl chloride is important to outline to inform instances of incidental releases, for example by spills and leaks.

3.4.3.1 Biosolids

Sludge is defined as the solid, semi-solid, or liquid residue generated by wastewater treatment processes. The term, “biosolids” refers to treated sludge that meet the EPA pollutant and pathogen requirements for land application and surface disposal (40 CFR 503) (U.S. EPA, 1993).

Vinyl chloride transport to terrestrial environments from the application of municipal biosolids is not expected to be a significant pathway, as removal of vinyl chloride in WWTP processes is expected to be dominated by stripping to air (see Section 3.5.3). In industrial settings, manufacturing byproduct solutions of vinyl chloride are stripped of volatile organics (including vinyl chloride) prior to being treated with activated sludge (ATSDR, 2024). Destruction of vinyl chloride by incineration is also recommended (ATSDR, 2024; NLM, 2023a) and is discussed in Section 3.5.1. By virtue of its solubility and log K_{OC}, vinyl chloride sorbed to solids in biosolids is expected to desorb readily and become mobile in areas receiving biosolids.

Vinyl chloride exposure may occur from landfill disposal of sludge from PVC manufacturing: EPA (1976) measured vinyl chloride monomer concentrations in PVC polymerization and processing sludges from three PVC plants and associated landfills representing common processing and disposal practices of the mid-1970s. Sludge concentrations ranged from 7 to 520 ppm ww (20 to 1,260 ppm dry weight [dw]). While these studies demonstrate possible routes for vinyl chloride release via biosolids to land pathways, they were conducted prior to the efforts made by the PVC industry to reduce vinyl chloride monomer levels in both finished PVC products and processing wastes headed to landfills. Therefore, they are not likely representative of current vinyl chloride concentrations in industrial sludge. Vinyl chloride was not included as an analyte in the most recent Targeted National Sewage Sludge Survey (U.S. EPA, 2009).

3.4.3.2 Soil

Vinyl chloride may enter soil through anticipated releases, migration of landfill leachate, and releases from spills and leaks. As mentioned above, application of biosolids (see Section 3.4.3.1) and deposition from air (see Section 3.4.1.1) are not expected to be important sources of vinyl chloride in soil. Vinyl chloride may also form in anaerobic soils from the reductive dehalogenation of more highly-chlorinated ethylenes (*e.g.*, PCE, TCE; see Section 3.3.4.5).

The extent to which vinyl chloride released to soil will remain in soil depends on its adsorption affinity to the soil type (see Section 3.2.2). Based on vinyl chloride’s vapor pressure, much of the vinyl chloride released to soil is expected to volatilize rapidly to the atmosphere. Vinyl chloride that remains in soil may be subject to several competing processes dictating its fate in soil, including (1) volatilization from both wet and dry soil, (2) migration to groundwater, (3) limited sorption to organic solid fractions, and (4) aerobic and anaerobic biodegradation. Because of vinyl chloride’s tendency to volatilize from soil and to have moderate to rapid migration to groundwater, only a small portion of vinyl chloride is likely to be subject to biodegradation in soil. As discussed in Section 3.3.4.3, biodegradation rates can vary greatly depending on the conditions and microbial species present. Given the anticipated transport and biodegradation in soil systems alongside low historical releases to land, vinyl chloride is not expected to persist in soil environments.

3.4.3.3 Landfills

Vinyl chloride is considered a hazardous waste under Subtitle C of the Resource Conservation and Recovery Act (RCRA) (40 CFR 261.33). However, the polymer PVC is not currently listed as a hazardous waste under RCRA, therefore materials containing PVC may be disposed of in conventional landfills. Information gathered to-date suggests that typical conditions in landfill environments will tend not to drive vinyl chloride monomer release from polymerized form in PVC products: Mersiowsky et al., (2001) performed lysimeter experiments over four years to track the release of organics from PVC wiring and flooring under simulated landfill conditions and found no detectable degradation of the PVC polymer (based on molecular weight distribution), and no vinyl chloride monomer in lysimeter biogas. The authors noted that the operating conditions of the simulated landfill environment were not amendable to depolymerization processes for PVC, with negligible UV exposure and temperatures well below processing temperature for PVC (160 °C). Subsequent publications have reported similar conclusions (Mersiowsky, 2002a; Mersiowsky, 2002b). Vinyl chloride may also enter landfills from leaching of residual vinyl chloride monomer from PVC materials. However, given improvements in PVC manufacturing practices, this is not expected to contribute significantly to vinyl chloride concentrations in landfills (see Section 3.5.2 for additional discussion on vinyl chloride monomer release from PVC pipe). Because PVC materials are a primary use of vinyl chloride, EPA plans to bolster the analysis of their fate within landfills with the conclusion of systematic review.

Additionally, vinyl chloride may occur in landfills from contaminated biosolids and the biological reductive dehalogenation of more highly-chlorinated ethylenes (*e.g.*, PCE, TCE), especially in deeper, anaerobic landfill layers. Kromann et al., (1998) studied the degradation under methanogenic conditions of five chlorinated aliphatic compounds (including PCE and TCE) in leachate collected from eight landfills in Denmark: three of the leachates were able to degrade PCE and TCE, showing complete primary degradation of PCE within 5 to 10 days following a 5 to 10-day lag period. A follow-up study demonstrated the sequential dechlorination of PCE in three of the leachates, following the sequence presented in Figure 3-3. The rate of reductive dechlorination to vinyl chloride was found to correlate with the level of biodegradable organics present in the leachate: vinyl chloride was produced and subsequently degraded within 40 and 69 days in the leachates with biological oxygen demands (BODs) of 780 and 500 mg-O_2/L, respectively, whereas no formation of vinyl chloride was detected by about day 83 in the leachate with a BOD of 140 mg-O_2/L (Kromann et al., 1998).

Vinyl chloride in gas form can diffuse upwards in landfill soils and may degrade in the presence of methane and oxygen, conditions characteristic of topsoil layers in landfills with methanogenic activity. Scheutz and Kjeldsen (2005) studied the potential for gas-phase vinyl chloride and other chlorinated VOCs to migrate in soil under methane oxidizing conditions characteristic of landfill soil cover systems. The authors found that when fed to a column alongside TCE containing landfill soil supplied with an oxygen/methane counter gradient, vinyl chloride exhibited 74±6 percent degradation from a starting test concentration of 310 µg/L and a gas flux rate of 0.76 m^3 landfill gas-m^2/day (Scheutz and Kjeldsen, 2005). The same publication reported that no degradation of vinyl chloride was observed in anaerobic batch experiments conducted with the same landfill soil with CO_2 and methane-filled headspace at a 50:50 ratio by volume, highlighting the importance of redox conditions on the degree to which vinyl chloride may be degraded in upper landfill layers. Kjeldsen and Christensen (2001) modeled the distribution of vinyl chloride in landfill gas, leachate, and sorbed to solids using a Model for Organic

Chemicals in Landfills (MOCLA) run under both "traditional" mixed landfill and reduced organics landfill conditions. The authors reported that the distribution of vinyl chloride remaining in the landfill—especially between the aqueous/leachate and solid/sorbed phases—is dependent on the organic carbon content of the solid media. Additionally, removal of vinyl chloride is expected to occur primarily through volatilization/gas flow and biodegradation (contingent upon the presence of appropriate microbial consortia and conditions), with minimal (less than 1 percent) remaining in the landfill after 5 years (Kjeldsen and Christensen, 2001). Fractions of vinyl chloride that are not degraded in the landfill will volatilize and may cause areas of elevated atmospheric concentrations above landfill surfaces (ATSDR, 2024; Molton et al., 1987).

Overall, the presence of vinyl chloride in landfills from the COUs relevant to this risk evaluation is not expected to be significant. Molton et al., (1987) studied the presence of vinyl chloride in municipal landfills in California where there was no prior knowledge of vinyl chloride being disposed of. The authors concluded that the most likely source of vinyl chloride in the studied landfills was from the anaerobic biodegradation of more highly-chlorinated solvents (*e.g.*, TCE), as vinyl chloride was observed only where chlorinated solvents were present in the landfill. Because very limited amounts of vinyl chloride are directly disposed of to landfills, and most land disposals are to RCRA landfills, exposure routes stemming from landfills are not expected to be significant.

3.4.3.4 Groundwater

Vinyl chloride may occur in groundwater from the degradation of more highly-chlorinated ethylenes (see Section 3.3.4.5). Additionally, due to its water solubility and low-to-moderate tendency to sorb to organics in soil, vinyl chloride fractions that do not volatilize (*i.e.*, during releases to soil in large and/or continuous amounts) are expected to be mobile in soil and may be transported to groundwater. However, as soil releases are not expected to be common (see Section 2.3.1 of *Draft Scope of the Risk Evaluation for Vinyl Chloride*), this is expected to be a minor pathway in the overall fate and persistence of vinyl chloride.

Vinyl chloride fractions that migrate to groundwater systems may be subject to both anaerobic biodegradation (rates discussed in Section 3.3.4.4) and abiotic reductive dehalogenation. The degree of susceptibility of vinyl chloride to abiotic dehalogenation relies on the minerality of the anaerobic system: of those determined only with minerals characteristic of soil and aquifer systems, rates of 0.055 to 0.15 d^{-1}, 0.247 to 0.323 d^{-1}, 0.355 to 0.537 d^{-1}, and 0.358 to 0.555 d^{-1} were determined with Silawa loamy sand, montmorillonite, vermiculite, and biotite, respectively (Reaxys, 2023). Assuming first order kinetics, these equate to half-lives ranging from 1.25 to 12.6 days. Despite the short half-lives achieved in laboratory reductive dehalogenation studies, vinyl chloride has been observed in groundwater in several U.S. locations (ATSDR, 2024), and may be fed by the degradation of more highly-chlorinated ethylene plumes (see Section 3.3.4.5).

3.5 Persistence Potential of Vinyl Chloride

In the atmosphere, vinyl chloride is not expected to undergo significant direct photolysis and will instead react with photochemically produced hydroxyl radicals (·OH). Based on reported hydroxyl radical-mediated indirect photolysis half-lives, vinyl chloride straddles the criterion for persistence in the air compartment ($t_{1/2} > 2$ days; see Section 3.3.2.1). In surface water and sediments under environmentally relevant conditions, vinyl chloride is not susceptible to appreciable hydrolysis (see Section 3.3.1). The persistence of vinyl chloride fractions remaining in the surface water compartment is expected to be mediated by biodegradation: given the range of empirical aerobic biodegradation half-lives, vinyl chloride is expected to have moderate to high persistence ($t_{1/2}$ 60 to ≥ 180 days) in the surface water compartment under environmentally relevant conditions (see Section 3.3.4.1). As a highly volatile chemical with a log K_{OC} range of 1.75 to 2.95, vinyl chloride is not expected to occur in sediments resulting from COUs of interest (see Section 3.2.2). In soil under environmentally relevant conditions, vinyl chloride may be subject to volatilization, migration to groundwater, and possible biodegradation and sorption to organic solid fractions (see Section 3.4.3.2).

3.5.1 Destruction and Removal Efficiency

Destruction and removal efficiency is a percentage that represents the mass of a pollutant removed or destroyed in a thermal incinerator relative to the mass that entered the system. EPA requires that hazardous waste incineration systems destroy and remove at least 99.99 percent of each harmful chemical in the waste, including treated hazardous waste (46 FR 7684, January 23, 1981).

O'Mara et al., (1971) reported that under diffusion conditions (*i.e.*, vinyl chloride monomer fed directly to a burner rather than combusted pre-mixed with air) the greatest combustion temperature reached was 950 °C when atmospheric oxygen was not limiting. The authors approximated that under diffusion conditions that mimic an actual vinyl chloride monomer fire, the air directly above the vinyl chloride flame would contain about 27,000 ppm HCl, 58,100 ppm CO_2, 9,500 ppm of CO, 40 ppm of $COCl_2$, and trace vinyl chloride monomer (O'Mara, 1971).

The recommended destruction method for vinyl chloride disposal is by incineration at temperatures between 450 and 1,600 °C (ATSDR, 2024; NLM, 2023a). Because of this, vinyl chloride is expected to have high destruction efficiency when incinerated within the temperature range recommended for destruction.

3.5.2 Presence and Removal in Drinking Water Treatment

Drinking water in the United States typically comes from surface water (*i.e.*, lakes, rivers, reservoirs) and groundwater. The source water then flows to a treatment plant where it undergoes a series of water treatment steps before being dispersed to homes and communities. In the U.S., public water systems often use conventional treatment processes that include coagulation, flocculation, sedimentation, filtration, and disinfection, as required by law.

Vinyl chloride may enter drinking water sources by degradation of higher chloroethylenes in groundwater (see Section 3.3.4.5), and also from primarily fugitive (*e.g.*, from spills and leaks) releases to surface water and to soil leading to migration to groundwater. Additionally, vinyl chloride monomer may leach from PVC drinking water distribution pipes. Dressman and Mcfarren (1978) sampled water from five distribution systems in Arizona, Texas, California, and Oregon that employed PVC piping that was manufactured between 1964 and 1975. The authors found detectable vinyl chloride in three of the five systems, with concentrations ranging from less than 0.03 µg/L (LOD) to 1.4 µg/L.

In 1977 a regulatory threshold of 10 mg/kg residual vinyl chloride monomer in new PVC was imposed, with a subsequent threshold of 3.2 mg/kg. This lower threshold was set based on diffusion modeling results to limit concentrations of residual vinyl chloride monomer leached from PVC pipes to 10% of the Maximum Contaminant Level (MCL) of 0.002 mg/L regulated under the Safe Drinking Water Act (40 C.F.R. 141.61) (Borrelli et al., 2005). The EPA Office of Water released a Permeation and Leaching report in 2002 indicating that 55 percent of 53 water samples collected from PVC distribution pipes manufactured prior to 1977 had vinyl chloride concentrations greater than the vinyl chloride monomer MCL of 0.002 mg/L (U.S. EPA, 2002). Factors such as contact time, temperature, and pipe diameter (surface area-to-volume ratio) were found to impact vinyl chloride concentrations. However, the same document reported zero instances of vinyl chloride concentrations above the MCL from water samples taken from PVC distribution pipes manufactured post-1977. Walter et al., (2011) performed a time course leaching study with new Schedule 40 PVC and found no detectable vinyl chloride monomer in the water samples from days 0 to 13, though saw an increase over time to about 130 ng/L at one year, and about 300 ng/L by day 581 (limit of quantification [LOQ] 95 ng/L). The authors also found that there were no statistically significant differences between vinyl chloride concentrations leached from unmodified PVC and chlorinated PVC during a shorter leaching study. Additionally, the authors found that vinyl chloride was more readily detectable in water measurements when chlorinated, municipal water was the supply water, rather than unchlorinated well water. However, the authors hypothesized that the latter observation was more likely due to formation of vinyl chloride as a disinfection byproduct rather than leaching from the pipes, though there were no confirming studies provided (Walter et al., 2011).

Limited information was identified on the removal efficiency of vinyl chloride during drinking water treatment. Based on vinyl chloride's volatility indicated by its HLC and vapor pressure, it is expected that high removal may be obtained through aeration and stripping-based treatment processes. Studies employing advanced treatment technologies have reported some capacity for vinyl chloride removal. For example, Ainscough et al., (2021) found an initial rejection rate of 70.3 percent across a low-energy reverse osmosis filtration, though efficiency drastically decreased with fouling after 21 days. Because surface water is expected to contain negligible vinyl chloride due to small releases, volatilization processes, and supporting monitoring studies (see Section 3.4.2), drinking water originating from surface water is unlikely to contain elevated vinyl chloride concentrations. However, drinking water sourced from groundwater near areas of chlorinated ethylene contamination may experience elevated concentrations, especially when subsequent drinking water treatment is absent.

3.5.3 Removal in Wastewater Treatment

Wastewater treatment is performed to remove contaminants from wastewater using physical, biological, and chemical processes. Generally, municipal wastewater treatment facilities apply primary and secondary treatments. During the primary treatment, screens, grit chambers, and settling tanks are used to remove solids from wastewater. Secondary treatment processes remove organic matter in wastewater using biological treatment processes such as trickling filters or activated sludge. Sometimes an additional stage of treatment such as tertiary treatment is utilized to further clean water for additional protection using advanced treatment techniques (*e.g.*, ozonation, chlorination, disinfection).

Very little vinyl chloride is expected to be released to municipal WWTPs. Due to its high volatility, vinyl chloride is expected to be removed from wastewater via stripping. EPA leveraged the STPWIN model in EPI Suite^{TM} to estimate removal efficiency of vinyl chloride from wastewater at a conventional treatment plant. Assuming negligible biodegradation by inputting a biodegradation half-life of 10,000 hours, STPWIN yielded a total removal 91.54 percent, with approximately 89 percent of the removal attributable to losses to stripping during aeration (U.S. EPA, 2017). Removal may be greater with the addition of contributions from biodegradation (see Section 3.3.4).

3.6 Bioaccumulation Potential of Vinyl Chloride

Information on bioconcentration and bioaccumulation in aquatic and terrestrial organisms is important to understanding the behavior of vinyl chloride in the environment and are a key component in assessing its risk to all living organisms, including humans.

Vinyl chloride is not expected to bioconcentrate or bioaccumulate significantly in aquatic organisms. Two empirical bioconcentration factors (BCF) were identified: a BCF of 40 was found in green algae (*Chlorella fusca*) (ATSDR, 2024; ECHA, 2023a; NLM, 2023a; OECD, 2001), and BCF less than 10 in golden ide (*Leuciscus idus melanotus*) (ATSDR, 2024; ECHA, 2023a; NLM, 2023a; OECD, 2001). No empirical bioaccumulation factor (BAF) values were identified. Because few BCF studies and no BAF studies were identified (see Table 3-2), the BCFBAF model of EPI Suite^{TM} v 4.11 was leveraged to fill aquatic bioaccumulation data gaps for screening purposes. Supporting evidence from empirical BCFs, BAFs of 2.31, 2.48, 3.17 L/kg were obtained for lower, middle, and upper trophic levels using the Arnot-Gobas method of the BCFBAF model (U.S. EPA, 2017). EPA identified no bioaccumulation or bioconcentration data for terrestrial organisms from databases or previously conducted assessments. Taken together with the expected release patterns and rapid partitioning to air, trophic transfer and exposures to humans from the consumption of animals are not expected to be significant pathways.

3.7 Overall Fate and Transport of Vinyl Chloride

EPA reviewed trusted databases and previously conducted assessments to identify information on fate endpoints for vinyl chloride that inform risk evaluation problem formulation. Specifically, this information was analyzed to characterize transport and partitioning pathways, identify environmental persistence potential, and assess bioaccumulation potential of vinyl chloride.

Intermedia Transport and Partitioning Behavior of Vinyl Chloride

The magnitude of the partitioning coefficients identified for vinyl chloride (Table 3-3) suggest that vinyl chloride will exist primarily in air and water in the environment. Vinyl chloride has a vapor pressure of 2,550 mmHg at 20 °C (ECHA, 2023a) indicating that vinyl chloride will exist predominantly as a free gas in the atmosphere, and dry deposition is unlikely to be an important process. This is consistent with the estimated octanol:air partition coefficient of 25.4 (U.S. EPA, 2017).

With a HLC of 0.0278 atm·m^3/mol at 24.8 °C (PhysProp, 2023), vinyl chloride is also expected to be volatile from surface water. While volatile, vinyl chloride also has considerable water solubility (9,150 mg/L at 20.5 °C (ECHA, 2023a; Reaxys, 2023)) consistent with its polarity and small molecular size. Sorption to organics present in sediment and suspended and dissolved solids present in water is unlikely to be a dominant pathway given the range of log K_{OC} values identified to date (Table 3-2). Vinyl chloride's solubility along with its log K_{OC} suggests that vinyl chloride that occurs in soil will exhibit mobility and may be transported through the vadose zone to groundwater.

Preliminary Media Assessments to Inform Problem Formulation

Preliminary media assessments were conducted to inform problem formulation for the risk evaluation of vinyl chloride, and to identify major and minor media in which vinyl chloride is expected to occur: due to vinyl chloride's physical and chemical properties driving its ready partitioning to air, as well as the vast majority (>98 %) of the TRI releases being reported to air, the air compartment is expected to be a major compartment of interest. Surface water and soil are expected to be minor compartments: vinyl chloride that remains in each of these media is expected to persist variably, moderated by biodegradation that is dependent on environmental conditions (*e.g.*, electron donors, oxygen levels, minerality). However, occurrences of vinyl chloride in surface water and soil are expected to be minimal as supported by monitoring and TRI release data. Biosolids, sediments, groundwater, and biota are expected to be minor compartments in the evaluation of vinyl chloride due to negligible releases and/or negligible partitioning to these media. The following subsections summarize the preliminary media assessments for this draft scope.

Air and Atmosphere

According to reporting to the TRI database, the majority of reported vinyl chloride releases are to air. Additionally, it is expected that vinyl chloride released to surface water and WWTPs will rapidly volatilize to the air compartment. In the atmosphere, vinyl chloride is expected to persist with a half-life range from 1.27 to 2.71 days (mean of 1.84 days) assuming a $\cdot$OH concentration of 1.5×10^6 $\cdot$OH/cm^3

and 12 hours of sunlight (see Sections 3.3.2.1 and 3.4.1.1) (OECD, 2001; ECHA, 2023a; NLM, 2023a; NIST, 2023; ATSDR, 2024).

In indoor air, vinyl chloride in gas phase is expected to be more persistent as compared to outdoor environments. Indoor environments have fewer physical transport drivers (*e.g.*, advection by wind and atmospheric flows) as well as less sunlight and subsequently lower concentrations of hydroxyl radicals. Therefore, vinyl chloride transformation rates are expected to be slow in indoor air. Vapor intrusion, however, is not expected to be a dominant pathway introducing vinyl chloride to indoor environments (see Section 3.4.1.2).

Aquatic Environments

Monitoring data from the Water Quality Portal indicate negligible instances of vinyl chloride in surface waters (see Section 3.4.2). Vinyl chloride may enter surface waters through anticipated releases, migration of landfill leachate, and releases from spills and leaks. Vinyl chloride is not expected to undergo wet or dry deposition (see Section 3.4.1.1). Vinyl chloride may also form in anaerobic media from the reductive dehalogenation of more highly-chlorinated ethylene contaminants (*e.g.*, PCE, TCE; see Section 3.3.4.5).

While vinyl chloride present in surface water is expected to volatilize appreciably, some fractions may remain dissolved in the aqueous phase and adsorbed to organics found in suspended solids, as indicated by the log K_{OC} values presented in Table 3-2. In surface water, vinyl chloride is expected to have moderate to high persistence. Because hydrolysis of vinyl chloride is negligible, its fate in water is expected to be primarily mediated by biodegradation processes.

One ready biodegradability test (OECD 301D) indicates vinyl chloride is not readily biodegradable, reporting a degradation rate of 16 percent over 28 days (ECHA, 2023a; NITE, 2023; NLM, 2023a). An additional CO_2 evolution study employing a municipal activated sludge inoculum reported a mineralization rate of 21.5 percent over 5 days (ECHA, 2023a; OECD, 2001). Anaerobic biodegradation rates range from a half-life of 70 days with groundwater inoculum, to 10 percent over 106 days in water under methanogenic conditions following a 50-day lag period (ECHA, 2023a; NLM, 2023a; Reaxys, 2023). The degree of vinyl chloride biodegradation in aqueous systems is therefore expected to vary with microbial community and environmental conditions. Despite not being readily biodegradable, vinyl chloride is not widely or frequently detected in aquatic environments, likely due to minimal releases to water and its tendency to volatilize rapidly.

No empirical data on vinyl chloride adsorption to sediment were identified. Based on empirical soil log K_{OC} values, however, vinyl chloride in the water column is not expected to partition significantly to organics in sediment, though it may be transported by diffusion and advection processes to sediment pore water. Given the range of both aerobic and anaerobic biodegradation rates identified in sediment and groundwater/sediment microcosms, vinyl chloride may exhibit a range of persistence behaviors dependent on the microbial community, redox conditions, and exposure history of the area to chlorinated solvents (*i.e.*, adaptation). However, as indicated by fugacity modeling (see Section 3.2.2) and identified monitoring data (see Section 3.4.2), vinyl chloride is not likely to be present in sediments.

Terrestrial Environments

Vinyl chloride may enter terrestrial environments via the disposal of industrial processing wastes, the degradation of higher chlorinated ethylenes (see Section 3.3.4.5), and incidental spills and leaks. Because the majority of reported releases are to air (see Section 3.2.2), and releases to soil media are expected to volatilize rapidly, terrestrial environments and processes are not expected to be significant to the evaluation of vinyl chloride. However, terrestrial fate of vinyl chloride is important to outline to inform instances of incidental releases, for example by fugitive spills and leaks.

Vinyl chloride may be subject to several competing processes dictating its fate in soil, including, (1) volatilization from both wet and dry soil, (2) moderate to rapid migration to groundwater, (3) limited sorption to organic solid fractions, and (4) limited aerobic and anaerobic biodegradation. Two sources were identified reporting log K_{OC} values for vinyl chloride. The first reported a log K_{OC} value of 1.75, but without additional detail on materials or methods (NLM, 2023a; OECD, 2001). The second is an empirical study following OECD 106 guidelines that investigated seven low-OC, natural clayey till soils from Denmark, reporting log K_{oc} values ranging from 2.38 to 2.95 (mean 2.70) (ATSDR, 2024). Because of vinyl chloride's large tendency to volatilize from soil and the possibility of some migration to groundwater, only a small portion of vinyl chloride is likely to be subject to biodegradation in soil. As discussed above, biodegradation rates can vary greatly depending on the conditions and microbial species present. Given the anticipated transport and biodegradation in soil systems, vinyl chloride is expected to have low to moderate persistence in soil.

Vinyl chloride present in groundwater systems is likely primarily due to the reductive dehalogenation of chlorinated solvents such as PCE and TCE (see Section 3.3.4.5). Vinyl chloride in groundwater may be subject to both anaerobic biodegradation and abiotic reductive dehalogenation. The degree of susceptibility of vinyl chloride to abiotic dehalogenation relies on the minerality of the anaerobic system, with estimated half-lives ranging from 1.25 to 12.6 days (Reaxys, 2023). Despite the short half-lives achieved in laboratory reductive dehalogenation studies, vinyl chloride has been observed in groundwater in several U.S. locations (ATSDR, 2024).

Volatility of vinyl chloride is expected to drive its removal in WWTPs (WWTPs). Results from the STPWIN model of EPI Suite™ v 4.11 predict that approximately 89 percent of vinyl chloride will be removed via losses to air stripping assuming negligible removal due to biodegradation (U.S. EPA, 2017). Negligible amounts of vinyl chloride are expected to partition to sludge during wastewater treatment, therefore vinyl chloride transport to terrestrial environments from the application of municipal biosolids is not expected to be a significant pathway (see Section 3.4.3.1).

Vinyl chloride may occur in landfills from illegal dumping or from the biological reductive dehalogenation of more highly-chlorinated ethylenes (*e.g.*, PCE, TCE), especially in deep, anaerobic landfill layers. Kromann et al., (1998) demonstrated that vinyl chloride may form and be degraded within the time frame of weeks to months, though is highly dependent on landfill characteristics. Vinyl chloride in gas form can also diffuse upwards in landfill soils and may degrade in the presence of methane and oxygen, conditions characteristic of topsoil layers in landfills with methanogenic activity (Scheutz and Kjeldsen, 2005). Fractions of vinyl chloride that are not degraded in the landfill may volatilize and may cause areas of elevated atmospheric concentrations above landfill surfaces (ATSDR, 2024; Molton et al., 1987). Because vinyl chloride in landfills is unlikely to occur from the COUs of interest, landfill pathways are not expected to be significant in subsequent risk analyses.

Bioaccumulation Potential

Vinyl chloride is not expected to bioconcentrate or bioaccumulate significantly in aquatic organisms. Two empirical bioconcentration factors (BCF) were identified: a BCF of 40 was found in green algae (*Chlorella fusca*) (ATSDR, 2024; ECHA, 2023a; NLM, 2023a; OECD, 2001), and BCF less than 10 in golden ide (*Leuciscus idus melanotus*) (ATSDR, 2024; ECHA, 2023a; NLM, 2023a; OECD, 2001). Supporting evidence from empirical BCFs, BAFs of 2.31, 2.48, 3.17 L/kg were obtained for lower, middle, and upper trophic levels using the Arnot-Gobas method of the BCFBAF model (U.S. EPA, 2017). EPA identified no bioaccumulation or bioconcentration data for terrestrial organisms from databases or previously conducted assessments.

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APPENDICES

Appendix A COMPARTMENT HALF-LIVES USED IN FUGACITY MODEL SENSITIVITY ANALYSIS

As discussed in Section 3.1.1, EPA leveraged a fugacity modeling approach to inform how vinyl chloride is expected to be distributed in the environment. Because systematic review and data quality evaluation steps are not yet complete, a sensitivity analysis was conducted to gauge a range of scenarios by varying compartment half-lives ($t_{1/2}$), and tendency to adsorb to organic carbon (varying log K_{OC}): the minimum, mean, and maximum empirical half-lives of vinyl chloride transformation in soil, water, and sediment were assessed, as well as the minimum and maximum log $K_{OC.}$ With the information gathered to date from trusted databases and previously conducted assessments, it is expected that the half-lives in typical surface water, soil, and sediments will be largely mediated by biodegradation, therefore the range and mean half-lives for each of these compartments was derived from available biodegradation data from which a first-order half-live was calculated using Equation 3-1. For the purposes of this exercise, both rates determined with non-adapted and pre-exposed (assumed some adaptation) were used, as adaptation due to exposure to vinyl chloride and/or other chlorinated solvents is not uncommon in several scenarios where vinyl chloride releases may be expected (*i.e.*, fugitive releases near industrial areas).

The following tables present the biodegradation studies and their associated calculated first order half-lives, as well as the range and mean of the half-lives in each media used in the fugacity model sensitivity analysis. In instances where multiple biodegradation values were extracted from one source (*e.g.*, from replicates, presented as a range), half-lives were calculated for each quantitative biodegradation value provided. While this is not ideal for determining central tendencies, this allows for capturing half-life extrema for the sensitivity analysis.

Table_Apx A-1 presents the available biodegradation studies conducted in aqueous systems. For the purposes of the fugacity sensitivity analysis, only the values collected under aerobic conditions (*i.e.*, Mechanism = Aerobic biodegradation) were included in the range and mean calculations. This was because surface waters were assumed to be aerobic.

Table_Apx A-1. Calculated Half-Lives from Biodegradation Studies in Water Following First-Order Kinetics

Mechanism	Value	$t_{1/2}$ (h)[a]	f_{VC_remain}	time, *t* (h)	Reference(s)
Aerobic biodegradation (water)	21.5% over 5 days (CO_2 Evolution) at 0.05 mg/L test substance concentration, with municipal activated sludge inoculum, adaptation not specified	343.61	0.785	5	OECD (2001), ECHA (2023a)
Aerobic biodegradation (water)	16% over 28 days (OECD 301D) at 2.04 test substance concentration; with sludge inoculum, adaptation not specified	2671.56	0.84	28	NITE (2023), ECHA (2023a), NLM (2023a)

Mechanism	Value	$t_{1/2}$ (h)[a]	f_{VC_remain}	time, t (h)	Reference(s)
Aerobic biodegradation (water)	22% over 28 days (CO_2 Evolution), with municipal activated sludge inoculum; some adaptation	1874.72	0.78	28	ECHA (2023c)
Anaerobic biodegradation (water)	10% over 106 days following a 50-day lag at 2.6 × 10-4 mg/L test substance concentration in groundwater containing H2 and acetate, under methanogenic conditions; adaptation likely due to media exposure to vinyl chloride	16736.50	0.9	106	Reaxys (2023)
Anaerobic biodegradation (water)	$t_{1/2}$ = 70 days at 0.4 mg/L test substance concentration, with groundwater bacteria inoculum, adaptation not specified	1680			ECHA (2023a), NLM (2023a)
Anaerobic biodegradation (water)	$t_{1/2}$ = 110 days; study details not specified	2640			NLM (2023a)
Half-life summary[b]					
	mean (h)	1629.96			
	min (h)	343.61			
	max (h)	2671.56			

[a] Calculated using a first-order approximation, described by Equation 3-1

[b] Summary statistics and values used in fugacity model only from aerobic studies (first four rows), as surface waters were assumed to be aerobic.

Table_Apx A-2 presents the biodegradation studies conducted with soil media. For the purposes of the fugacity sensitivity analysis, both aerobic and anaerobic values were included in the range and mean calculations. This is because it was assumed that soil environments contain a gradient of oxygen availability, thus including both aerobic and anaerobic conditions will help to capture a range of conditions with the sensitivity analysis. Similarly, studies using soil and water from a shallow aquifer were included here.

Table_Apx A-2. Calculated Half-Lives from Biodegradation Studies in Soil Following First-Order Kinetics

Mechanism	Value	$t_{1/2}$ (h)[a]	f_{VC_remain}	time, t (h)	Reference(s)
Aerobic biodegradation (soil)	>99% over 108 days (transformation) and 65% over 108 days (mineralization) at 1 mg/L test substance concentration in a natural shallow aquifer soil/groundwater microcosm, adaptation not specified	195.07	1.00E-04	2592	OECD (2001), ATSDR (2024) ECHA (2023a)
Aerobic biodegradation (soil)	>99% over 108 days (transformation) and 65% over 108 days (mineralization) at 1 mg/L test substance concentration in a natural shallow aquifer soil/groundwater microcosm, adaptation not specified	1711.37	0.35	2592	OECD (2001), ATSDR (2024) ECHA (2023a)
Aerobic biodegradation (soil)	1.456 µg/g soil/hour biodegradation in gas phase, incubated with soil from a landfill under methane oxidizing conditions	476.06			NLM (2023a)
Anaerobic biodegradation (soil)	$t_{1/2}$ = 4 weeks at 0.4 mg/L test substance concentration, in sand/water microcosm; adaptation not specified	672			ECHA (2023a), NLM (2023a)
Half-life summary					
	mean (h)	763.63			
	min (h)	195.07			
	max (h)	1711.37			

[a] Calculated using a first-order approximation, described by Equation 3-1.

Table_Apx A-3 presents the biodegradation studies conducted with sediment media. For the purposes of the fugacity sensitivity analysis, both aerobic and anaerobic values were included in the range and mean calculations. This is because it was assumed that the conditions in sediment environments comprise both surface sediments and deeper anaerobic sediments, and including both aerobic and anaerobic conditions will help to capture this range with the sensitivity analysis. Additionally, studies using media from a variety of locations (including aquifers) were included to capture a range of adaptation conditions, mineralities, organic matter contents, and electron donors. With the completion of systematic review, the studies selected for fugacity modeling are expected to be refined as their data undergoes quality control review.

Table_Apx A-3. Calculated Half-Lives from Biodegradation Studies with Sediment Following

1510 **First-Order Kinetics**

Mechanism	Value	$t_{1/2}$ (h)[a]	f_{VC_remain}	time, t (h)	Reference(s)
Aerobic biodegradation (groundwater microcosms)	22% to 39% over 84 hours (mineralization) at approx. 1.13 mg/L test substance concentration in natural aquifer microcosm; some adaptation from chlorinated solvent and vinyl chloride contamination	234.34	7.80E-01	84	Reaxys (2023), ATSDR (2024)
Aerobic biodegradation (groundwater microcosms)	22% to 39% over 84 hours (mineralization) at approx. 1.13 mg/L test substance concentration in natural aquifer microcosm; some adaptation from chlorinated solvent and vinyl chloride contamination	117.79	6.10E-01	84	Reaxys (2023), ATSDR (2024)
Aerobic biodegradation (groundwater microcosms)	>99% over 57 days, and >99% over 204 days at 330 µg/L test substance concentration, in groundwater/sediment batch microcosms; adaptation likely due to media exposure to vinyl chloride	205.9	1.00E-02	1368	NLM (2023a)
Aerobic biodegradation (groundwater microcosms)	>99% over 57 days, and >99% over 204 days at 330 µg/L test substance concentration, in groundwater/sediment batch microcosms; adaptation likely due to media exposure to vinyl chloride	736.92	1.00E-02	4896	NLM (2023a)
Anaerobic biodegradation (groundwater microcosms)	15% to 34% over 84 hours, and 2.8% to 4.6% over 84 hours (mineralization) at approx. 1.13 mg/L test substance concentration, in natural aquifer microcosm, amended with Fe(III) and unamended, respectively; some adaptation from media exposure to chlorinated solvents and vinyl chloride	358.26	8.50E-01	84	Reaxys (2023), ATSDR (2024)

Mechanism	Value	$t_{1/2}$ (h)[a]	f_{VC_remain}	time, t (h)	Reference(s)
Anaerobic biodegradation (groundwater microcosms)	15% to 34% over 84 hours, and 2.8% to 4.6% over 84 hours (mineralization) at approx. 1.13 mg/L test substance concentration, in natural aquifer microcosm, amended with Fe(III) and unamended, respectively; some adaptation from media exposure to chlorinated solvents and vinyl chloride	140.13	6.60E-01	84	Reaxys (2023), ATSDR (2024)
Anaerobic biodegradation (groundwater microcosms)	15% to 34% over 84 hours, and 2.8% to 4.6% over 84 hours (mineralization) at approx. 1.13 mg/L test substance concentration, in natural aquifer microcosm, amended with Fe(III) and unamended, respectively; some adaptation from media exposure to chlorinated solvents and vinyl chloride	2050.19	9.72E-01	84	Reaxys (2023), ATSDR (2024)
Anaerobic biodegradation (groundwater microcosms)	15% to 34% over 84 hours, and 2.8% to 4.6% over 84 hours (mineralization) at approx. 1.13 mg/L test substance concentration, in natural aquifer microcosm, amended with Fe(III) and unamended, respectively; some adaptation from media exposure to chlorinated solvents and vinyl chloride	1236.41	9.54E-01	84	Reaxys (2023), ATSDR (2024)
Anaerobic biodegradation (sediment)	5% to 44% over 37 days, and 8% to 100% over 37 days (mineralization) at 0.013 to 3.79 mg/L test substance concentration, in natural creek bed microcosm under methanogenic and Fe (III)-reducing conditions, respectively; some adaptation from former drum disposal area	11999.91	9.50E-01	888	Reaxys (2023), ATSDR (2024)

Mechanism	Value	$t_{1/2}$ (h)[a]	f_{VC_remain}	time, t (h)	Reference(s)
Anaerobic biodegradation (sediment)	5% to 44% over 37 days, and 8% to 100% over 37 days (mineralization) at 0.013 to 3.79 mg/L test substance concentration, in natural creek bed microcosm under methanogenic and Fe (III)-reducing conditions, respectively; some adaptation from former drum disposal area	1061.56	5.60E-01	888	Reaxys (2023), ATSDR (2024)
Anaerobic biodegradation (sediment)	5% to 44% over 37 days, and 8% to 100% over 37 days (mineralization) at 0.013 to 3.79 mg/L test substance concentration, in natural creek bed microcosm under methanogenic and Fe (III)-reducing conditions, respectively; some adaptation from former drum disposal area	7381.9	9.20E-01	888	Reaxys (2023), ATSDR (2024)
Anaerobic biodegradation (sediment)	5% to 44% over 37 days, and 8% to 100% over 37 days (mineralization) at 0.013 to 3.79 mg/L test substance concentration, in natural creek bed microcosm under methanogenic and Fe (III)-reducing conditions, respectively; some adaptation from former drum disposal area	53.46	1.00E-05	888	Reaxys (2023), ATSDR (2024)
Anaerobic biodegradation (sediment)	50% over 25 days and 100% over 19 days with 0.02 and 0.1 mg/L dissolved oxygen, respectively, at 0.65 mg test substance; vinyl chloride-oxidizing culture inoculum in microcosm with media from contaminated site; adapted	600			ATSDR (2024)

Mechanism	**Value**	**$t_{1/2}$ (h)**[a]	**f_{VC_remain}**	**time, t (h)**	**Reference(s)**
Anaerobic biodegradation (sediment)	50% over 25 days and 100% over 19 days with 0.02 and 0.1 mg/L dissolved oxygen, respectively, at 0.65 mg test substance; vinyl chloride-oxidizing culture inoculum in microcosm with media from contaminated site; adapted	27.45	1.00E-05	456	ATSDR (2024)
Anaerobic biodegradation (sediment)	98% and 21% over 70 days in Naval Air Station, and Naval Weapons Industrial Reserve Plant sediment microcosms, respectively; under methanogenic conditions; some adaptation with preexposure of media to chlorinated solvents	297.67	2.00E-02	1680	ECHA (2023a)
Anaerobic biodegradation (sediment)	98% and 21% over 70 days in Naval Air Station, and Naval Weapons Industrial Reserve Plant sediment microcosms, respectively; under methanogenic conditions; some adaptation with preexposure of media to chlorinated solvents	4940.08	7.90E-01	1680	ECHA (2023a)
Anaerobic biodegradation (groundwater microcosms)	100% over >100 days at 39 mg/L test substance concentration in groundwater with sediment microcosm under Fe-and SO_4^-reducing conditions; media from contaminated site	144.49	1.00E-05	2400	Reaxys (2023)
Anaerobic biodegradation (sediment)	40% over 20 hours at 31.2 mg/L test substance concentration, in brackish sediment microcosm supplemented with methanol; adapted inoculum	27.14	6.00E-01	20	Reaxys (2023)
Anaerobic biodegradation (sediment)	40% over 20 hours at 28.7 mg/L test substance concentration, in brackish sediment microcosm supplemented with H_2; adapted inoculum	27.14	6.00E-01	20	Reaxys (2023)

Mechanism	**Value**	**$t_{1/2}$ (h)[a]**	**f_{VC_remain}**	**time, t (h)**	**Reference(s)**
Anaerobic biodegradation (groundwater microcosms)	100% over 15 days in aquifer microcosm supplemented with methanol and C_2Cl_4; some adaptation with preexposure of media to chlorinated solvents	21.67	1.00E-05	360	Reaxys (2023)
Anaerobic biodegradation (groundwater microcosms)	100% over 14 weeks, and <20% over 14 weeks with and without supplemented e- donors, respectively, in aquifer microcosm; some adaptation with media from vinyl chloride-contaminated site	141.6	1.00E-05	2352	Reaxys (2023)
Anaerobic biodegradation (groundwater microcosms)	100% over 14 weeks, and <20% over 14 weeks with and without supplemented e- donors, respectively, in aquifer microcosm; some adaptation with media from vinyl chloride-contaminated site	7305.98	8.00E-01	2352	Reaxys (2023)
Half-life summary					
	mean (h)	1777.73			
	min (h)	21.67			
	max (h)	11999.91			

[a] Calculated using a first-order approximation, described by Equation 3-1.

Appendix B EPI SUITE™ MODEL OUTPUTS

This section presents the raw output from EPISuite™ (U.S. EPA, 2017). Please note that the sensitivity analysis described in Sections 3.1.1 are not captured in this section and are instead presented in Section 3.2.2.

EPI Suite Results For CAS 000075-01-4

```


                                              ENDKed
SMILES : C(=C)CL
CHEM  : Ethene, chloro-
MOL FOR: C2 H3 CL1
MOL WT : 62.50
------------------------------ EPI SUMMARY (v4.11) --------------------------
Physical Property Inputs:
Log Kow (octanol-water):  1.38
Boiling Point (deg C) :  -13.90
Melting Point (deg C) :  -153.84
Vapor Pressure (mm Hg) :  2550
Water Solubility (mg/L):  9150
Henry LC (atm-m3/mole) :  0.0278

KOWWIN Program (v1.68) Results:
===============================

Log Kow(version 1.69 estimate): 1.62

Experimental Database Structure Match:
Name    : VINYLCHLORIDE
CAS Num : 000075-01-4
Exp Log P: 1.46
Exp Ref : SAKURATANI,Y ET AL. (2007)

SMILES : C(=C)CL
CHEM  : Ethene, chloro-
MOL FOR: C2 H3 CL1
MOL WT : 62.50
-------+-----+--------------------------------------------+---------+--------
TYPE | NUM |    LOGKOW FRAGMENT DESCRIPTION     | COEFF | VALUE
-------+-----+--------------------------------------------+---------+--------
Frag | 1 | =CH2  [olefinic carbon]          | 0.5184 | 0.5184
Frag | 1 | =CH- or =C< [olefinc carbon]       | 0.3836 | 0.3836
Frag | 1 | -CL   [chlorine, olefinic attach]    | 0.4923 | 0.4923
Const |    | Equation Constant              |      | 0.2290
-------+-----+--------------------------------------------+---------+--------
Log Kow  =  1.6233




MPBPVP (v1.43) Program Results:
===============================
Experimental Database Structure Match:
Name    : VINYLCHLORIDE
CAS Num : 000075-01-4
Exp MP (deg C): -153.84
Exp BP (deg C): -13.8
Exp VP (mm Hg): 2.98E+03 (extrapolated)
```

```
(Pa  ): 3.97E+005
Exp VP (deg C): 25
Exp VP ref  : DAUBERT,TE & DANNER,RP (1985)

SMILES : C(=C)CL
CHEM  : Ethene, chloro-
MOL FOR: C2 H3 CL1
MOL WT : 62.50
------------------------ SUMMARY MPBPWIN v1.44 --------------------


Boiling Point:  3.97 deg C (Adapted Stein and Brown Method)

Melting Point: -132.70 deg C (Adapted Joback Method)
Melting Point: -111.35 deg C (Gold and Ogle Method)
Mean Melt Pt : -122.02 deg C (Joback; Gold,Ogle Methods)
Selected MP: -122.02 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: -13.90 deg C (user entered))
(MP not used for liquids)
VP: 2.87E+003 mm Hg (Antoine Method)
: 3.83E+005 Pa (Antoine Method)
VP: 2.67E+003 mm Hg (Modified Grain Method)
: 3.56E+005 Pa (Modified Grain Method)
VP: 2.59E+003 mm Hg (Mackay Method)
: 3.45E+005 Pa (Mackay Method)
Selected VP: 2.77E+003 mm Hg (Mean of Antoine & Grain methods)
: 3.7E+005 Pa (Mean of Antoine & Grain methods)



-------+-----+--------------------+----------+---------
TYPE | NUM | BOIL DESCRIPTION | COEFF  | VALUE
-------+-----+--------------------+----------+---------
Group | 1 | =CH2       |  16.44 |  16.44
Group | 1 | =CH-       |  27.95 |  27.95
Group | 1 | -Cl        |  34.08 |  34.08
*  |   | Equation Constant |     | 198.18
============+====================+==========+=========
RESULT-uncorr| BOILING POINT in deg Kelvin | 276.65
RESULT- corr | BOILING POINT in deg Kelvin | 277.13
| BOILING POINT in deg C    |  3.97
------------------------------------------------------

-------+-----+--------------------+----------+---------
TYPE | NUM | MELT DESCRIPTION | COEFF  | VALUE
-------+-----+--------------------+----------+---------
Group | 1 | =CH2       |  -4.32 |  -4.32
Group | 1 | =CH-       |  8.73 |  8.73
Group | 1 | -Cl        |  13.55 |  13.55
*  |   | Equation Constant |     | 122.50
============+====================+==========+=========
RESULT  | MELTING POINT in deg Kelvin | 140.46
| MELTING POINT in deg C    | -132.70
------------------------------------------------------



Water Sol from Kow (WSKOW v1.42) Results:
```

```
========================================

Water Sol: 9286 mg/L

Experimental Water Solubility Database Match:
Name    : VINYLCHLORIDE
CAS Num : 000075-01-4
Exp WSol : 8800 mg/L (25 deg C)
Exp Ref : DELASSUS,PT & SCHMIDT,DD (1981)

SMILES : C(=C)CL
CHEM  : Ethene, chloro-
MOL FOR: C2 H3 CL1
MOL WT : 62.50
---------------------------------- WSKOW v1.43 Results ------------------------
Log Kow (estimated) : 1.62
Log Kow (experimental): 1.46
Cas No: 000075-01-4
Name : VINYLCHLORIDE
Refer : SAKURATANI,Y ET AL. (2007)
Log Kow used by Water solubility estimates: 1.38 (user entered)

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.693-0.96 log Kow-0.0092(Tm-25)-0.00314 MW + Correction

Melting Pt (Tm) = -153.84 deg C (Use Tm = 25 for all liquids)

Correction(s):     Value
--------------------  -----
No Applicable Correction Factors

Log Water Solubility (in moles/L) : -0.828
Water Solubility at 25 deg C (mg/L): 9286



WATERNT Program (v1.01) Results:
===============================

Water Sol (v1.01 est): 4120.2 mg/L

Experimental Water Solubility Database Match:
Name    : VINYLCHLORIDE
CAS Num : 000075-01-4
Exp WSol : 8800 mg/L (25 deg C)
Exp Ref : DELASSUS,PT & SCHMIDT,DD (1981)

SMILES : C(=C)CL
CHEM  : Ethene, chloro-
MOL FOR: C2 H3 CL1
MOL WT : 62.50
-------+-----+--------------------------------------------+----------+---------
TYPE | NUM |  WATER SOLUBILITY FRAGMENT DESCRIPTION  | COEFF  | VALUE
-------+-----+--------------------------------------------+----------+---------
Frag | 1 | =CH2  [olefinic carbon]          |-0.4789  | -0.4789
Frag | 1 | =CH- or =C< [olefinc carbon]       |-0.3646  | -0.3646
Frag | 1 | -CL   [chlorine, olefinic attach]    |-0.5867  | -0.5867
Const |    | Equation Constant              |      | 0.2492
-------+-----+--------------------------------------------+---------+---------
Log Water Sol (moles/L) at 25 dec C =  -1.1810
```

```
Water Solubility (mg/L) at 25 dec C =  4120.2



ECOSAR Program (v1.11) Results:
===============================
ECOSAR Version 1.11 Results Page

SMILES : C(=C)CL
CHEM   : Ethene, chloro-
CAS Num:
ChemID1:
MOL FOR: C2 H3 CL1
MOL WT : 62.50
Log Kow: 1.623   (EPISuite Kowwin v1.68 Estimate)
Log Kow:      (User Entered)
Log Kow: 1.46    (PhysProp DB exp value - for comparison only)
Melt Pt: -153.84  (deg C, User Entered for Wat Sol estimate)
Melt Pt: -153.84  (deg C, PhysProp DB exp value for Wat Sol est)
Wat Sol: 7781    (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol: 9150    (mg/L, User Entered)
Wat Sol: 8800    (mg/L, PhysProp DB exp value)


--------------------------------------
Values used to Generate ECOSAR Profile
--------------------------------------
Log Kow: 1.623   (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 9150    (mg/L, User Entered)



--------------------------------------
ECOSAR v1.11 Class-specific Estimations
--------------------------------------
Vinyl/Allyl Halides
Predicted
ECOSAR Class                     Organism      Duration End Pt  mg/L (ppm)
=========================== ================== ======== ======  ==========
Vinyl/Allyl Halides    : Fish         96-hr   LC50    26.735
Vinyl/Allyl Halides    : Daphnid      48-hr   LC50    21.050
Vinyl/Allyl Halides    : Green Algae      96-hr   EC50    27.439
Vinyl/Allyl Halides    : Fish              ChV    14.782
Vinyl/Allyl Halides    : Daphnid             ChV     0.080
Vinyl/Allyl Halides    : Green Algae           ChV     5.049 !
Vinyl/Allyl Halides    : Fish (SW)      96-hr   LC50    20.124
Vinyl/Allyl Halides    : Mysid (SW)     96-hr   LC50    9.925
Vinyl/Allyl Halides    : Earthworm      14-day  LC50    84.587

=========================== ================== ======== ======  ==========
Neutral Organic SAR    : Fish         96-hr   LC50   111.889
(Baseline Toxicity)    : Daphnid        48-hr   LC50    61.360
: Green Algae     96-hr   EC50    39.585
: Fish              ChV    10.497
: Daphnid             ChV     5.432
: Green Algae           ChV     9.594

Note: * = asterisk designates: Chemical may not be soluble enough to
measure this predicted effect. If the effect level exceeds the
water solubility by 10X, typically no effects at saturation (NES)
```

```
are reported.

NOTE: ! = exclamation designates: The toxicity value was estimated through
application of acute-to-chronic ratios per methods outlined in
the ECOSAR Methodology Document provided in the ECOSAR Help Menu.


------------------------------
Class Specific LogKow Cut-Offs
------------------------------
If the log Kow of the chemical is greater than the endpoint specific cut-offs
presented below, then no effects at saturation are expected for those endpoints.

Vinyl/Allyl Halides:
-------------------
Maximum LogKow: 6.0 (Fish 96-hr LC50; Daphnid LC50; Mysid LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 5.0 (Fish (SW) 96-hr LC50)
Maximum LogKow: 6.0 (Earthworm LC50)
Maximum LogKow: 8.0 (ChV)

Baseline Toxicity SAR Limitations:
---------------------------------
Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)





HENRYWIN (v3.20) Program Results:
=============================

Bond Est : 4.44E-002 atm-m3/mole (4.50E+003 Pa-m3/mole)
Group Est: 5.60E-002 atm-m3/mole (5.68E+003 Pa-m3/mole)

SMILES : C(=C)CL
CHEM   : Ethene, chloro-
MOL FOR: C2 H3 CL1
MOL WT : 62.50
--------------------------- HENRYWIN v3.21 Results --------------------------

Experimental Database Structure Match:
Name    : VINYLCHLORIDE
CAS Num : 000075-01-4
Exp HLC : 2.78E-02 atm-m3/mole (2.82E+003 Pa-m3/mole)
Temper  : 24 deg C
Exp Ref : GOSSETT,JM (1987)

----------+---------------------------------------------+---------+----------
CLASS |   BOND CONTRIBUTION DESCRIPTION      | COMMENT | VALUE
----------+---------------------------------------------+---------+----------
HYDROGEN |  3 Hydrogen to Carbon (olefinic) Bonds  |     | -0.3014
FRAGMENT |  1 Cd-CL                    |     | 0.0426
FRAGMENT |  1 Cd=Cd                    |     | 0.0000
----------+---------------------------------------------+---------+----------
RESULT  |  BOND ESTIMATION METHOD for LWAPC VALUE  | TOTAL | -0.259
----------+---------------------------------------------+---------+----------
HENRYs LAW CONSTANT at 25 deg C = 4.44E-002 atm-m3/mole
```

```
= 1.81E+000 unitless
= 4.50E+003 Pa-m3/mole

--------+-----------------------------------------------+------------+--------
|    GROUP CONTRIBUTION DESCRIPTION     |  COMMENT | VALUE
--------+-----------------------------------------------+------------+--------
|      1 Cd-H2              |      | -0.41
|      1 CdH (CL)             |      | 0.05
--------+-----------------------------------------------+------------+--------
RESULT | GROUP ESTIMATION METHOD for LOG GAMMA VALUE |  TOTAL  | -0.36
--------+-----------------------------------------------+------------+--------
HENRYs LAW CONSTANT at 25 deg C = 5.60E-002 atm-m3/mole
= 2.29E+000 unitless
= 5.68E+003 Pa-m3/mole


For Henry LC Comparison Purposes:
Exper Database: 2.78E-02 atm-m3/mole (2.82E+003 Pa-m3/mole)
User-Entered Henry LC: 2.780E-002 atm-m3/mole (2.817E+003 Pa-m3/mole)
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 6.831E-003 atm-m3/mole (6.921E+002 Pa-m3/mole)
VP:  2.55E+003 mm Hg (source: User-Entered)
WS:  9.15E+003 mg/L (source: User-Entered)



Log Octanol-Air (KOAWIN v1.10) Results:
======================================

Log Koa: 1.324

SMILES : C(=C)CL
CHEM  : Ethene, chloro-
MOL FOR: C2 H3 CL1
MOL WT : 62.50
--------------------------- KOAWIN v1.10 Results --------------------------

Log Koa (octanol/air) estimate: 1.324
Koa (octanol/air) estimate: 21.11
Using:
Log Kow: 1.38 (user entered)
HenryLC: 0.0278 atm-m3/mole (user entered)
Log Kaw: 0.056 (air/water part.coef.)

LogKow : 1.46 (exp database)
LogKow : 1.62 (KowWin estimate)
Henry LC: 0.0278 atm-m3/mole (exp database)
Henry LC: 0.0444 atm-m3/mole (HenryWin bond estimate)

Log Koa (octanol/air) estimate: 1.361 (from KowWin/HenryWin)



BIOWIN (v4.10) Program Results:
==============================
SMILES : C(=C)CL
CHEM  : Ethene, chloro-
MOL FOR: C2 H3 CL1
MOL WT : 62.50
--------------------------- BIOWIN v4.10 Results ----------------------------
```

```
Biowin1 (Linear Model Prediction)  : Biodegrades Fast
Biowin2 (Non-Linear Model Prediction): Biodegrades Fast
Biowin3 (Ultimate Biodegradation Timeframe): Weeks
Biowin4 (Primary Biodegradation Timeframe): Days-Weeks
Biowin5 (MITI Linear Model Prediction)  : Does Not Biodegrade Fast
Biowin6 (MITI Non-Linear Model Prediction): Does Not Biodegrade Fast
Biowin7 (Anaerobic Model Prediction): Biodegrades Fast
Ready Biodegradability Prediction: NO

------+-----+--------------------------------------------+---------+---------
TYPE | NUM |    Biowin1 FRAGMENT DESCRIPTION     | COEFF | VALUE
------+-----+--------------------------------------------+---------+---------
Frag | 1 | Aliphatic chloride  [-CL]         | -0.1114 | -0.1114
MolWt| * | Molecular Weight Parameter         |     | -0.0298
Const| * | Equation Constant               |     | 0.7475
============+============================================+=========+=========
RESULT  |  Biowin1 (Linear Biodeg Probability)   |     | 0.6064
============+============================================+=========+=========


------+-----+--------------------------------------------+---------+---------
TYPE | NUM |    Biowin2 FRAGMENT DESCRIPTION     | COEFF | VALUE
------+-----+--------------------------------------------+---------+---------
Frag | 1 | Aliphatic chloride  [-CL]         | -1.8528 | -1.8528
MolWt| * | Molecular Weight Parameter         |     | -0.8875
============+============================================+=========+=========
RESULT  | Biowin2 (Non-Linear Biodeg Probability)  |     | 0.5667
============+============================================+=========+=========

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+--------------------------------------------+---------+---------
TYPE | NUM |    Biowin3 FRAGMENT DESCRIPTION     | COEFF | VALUE
------+-----+--------------------------------------------+---------+---------
Frag | 1 | Aliphatic chloride  [-CL]         | -0.1732 | -0.1732
MolWt| * | Molecular Weight Parameter         |     | -0.1381
Const| * | Equation Constant               |     | 3.1992
============+============================================+=========+=========
RESULT  | Biowin3 (Survey Model - Ultimate Biodeg) |     | 2.8879
============+============================================+=========+=========

------+-----+--------------------------------------------+---------+---------
TYPE | NUM |    Biowin4 FRAGMENT DESCRIPTION     | COEFF | VALUE
------+-----+--------------------------------------------+---------+---------
Frag | 1 | Aliphatic chloride  [-CL]         | -0.1006 | -0.1006
MolWt| * | Molecular Weight Parameter         |     | -0.0902
Const| * | Equation Constant               |     | 3.8477
============+============================================+=========+=========
RESULT  |  Biowin4 (Survey Model - Primary Biodeg) |     | 3.6570
============+============================================+=========+=========

Result Classification:  5.00 -> hours   4.00 -> days  3.00 -> weeks
 (Primary & Ultimate)  2.00 -> months  1.00 -> longer

------+-----+--------------------------------------------+---------+---------
TYPE | NUM |    Biowin5 FRAGMENT DESCRIPTION     | COEFF | VALUE
------+-----+--------------------------------------------+---------+---------
Frag | 1 | Aliphatic chloride  [-CL]         | 0.0174 | 0.0174
Frag | 3 | -C=CH [alkenyl hydrogen]          | -0.0058 | -0.0175
```

```
MolWt| * | Molecular Weight Parameter        |      | -0.0986
Const| * | Equation Constant             |      | 0.5544
============+=============================================+=========+=========
RESULT  | Biowin5 (MITI Linear Biodeg Probability) |     | 0.4557
============+=============================================+=========+=========

------+-----+---------------------------------------------+---------+---------
TYPE | NUM |    Biowin6 FRAGMENT DESCRIPTION     | COEFF | VALUE
------+-----+---------------------------------------------+---------+---------
Frag | 1 | Aliphatic chloride  [-CL]         | -0.6392 | -0.6392
Frag | 3 | -C=CH [alkenyl hydrogen]          | -0.0921 | -0.2764
MolWt| * | Molecular Weight Parameter        |      | -1.0812
============+=============================================+=========+=========
RESULT  |Biowin6 (MITI Non-Linear Biodeg Probability)|     | 0.4171
============+=============================================+=========+=========

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable


------+-----+---------------------------------------------+---------+---------
TYPE | NUM |    Biowin7 FRAGMENT DESCRIPTION     | COEFF | VALUE
------+-----+---------------------------------------------+---------+---------
Frag | 1 | Aliphatic chloride  [-CL]         | -0.0147 | -0.0147
Frag | 3 | -C=CH [alkenyl hydrogen]          | -0.0735 | -0.2206
Const| * | Equation Constant             |      | 0.8361
============+=============================================+=========+=========
RESULT  |  Biowin7 (Anaerobic Linear Biodeg Prob)  |     | 0.6009
============+=============================================+=========+=========

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)
----------------------------------------------
Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey
model) result is "weeks" or faster (i.e. "days", "days to weeks", or
"weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then
the prediction is YES (readily biodegradable). If this condition is not
satisfied, the prediction is NO (not readily biodegradable). This method
is based on application of Bayesian analysis to ready biodegradation data
(see Help). Biowin5 and 6 also predict ready biodegradability, but for
degradation in the OECD301C test only; using data from the Chemicals
Evaluation and Research Institute Japan (CERIJ) database.




BioHCwin (v1.01) Program Results:
==============================
SMILES : C(=C)CL
CHEM  : Ethene, chloro-
MOL FOR: C2 H3 CL1
MOL WT : 62.50
-------------------------- BioHCwin v1.01 Results ---------------------------

NO Estimate Possible ... Structure NOT a Hydrocarbon
(Contains atoms other than C, H or S (-S-))
```

```
AEROWIN Program (v1.00) Results:
===============================
Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 3.4E+005 Pa (2.55E+003 mm Hg)
Log Koa (Koawin est ): 1.324
Kp (particle/gas partition coef. (m3/ug)):
Mackay model      : 8.82E-012
Octanol/air (Koa) model: 5.18E-012
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model   : 3.19E-010
Mackay model      : 7.06E-010
Octanol/air (Koa) model: 4.14E-010


AOP Program (v1.92) Results:
===========================
SMILES : C(=C)CL
CHEM  : Ethene, chloro-
MOL FOR: C2 H3 CL1
MOL WT : 62.50
------------------- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) --------
Hydrogen Abstraction    =  0.0000 E-12 cm3/molecule-sec
Reaction with N, S and -OH =  0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds  =  0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =  5.5230 E-12 cm3/molecule-sec
Addition to Aromatic Rings =  0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings  =  0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant =  5.5230 E-12 cm3/molecule-sec
HALF-LIFE =   1.937 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE =  23.240 Hrs
------------------- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) -----------
OVERALL OZONE Rate Constant =   0.025025 E-17 cm3/molecule-sec
HALF-LIFE =   45.794 Days (at 7E11 mol/cm3)

Experimental Database Structure Match:
Chem Name : VINYLCHLORIDE
CAS Number: 000075-01-4
Exper OH rate constant  : 6.96 E-12 cm3/molecule-sec
Exper OH Reference: KWOK,ESC & ATKINSON,R (1994)
Exper Ozone rate constant: 2.46 E-19 cm3/molecule-sec
Exper NO3 rate constant : 4.85 E-16 cm3/molecule-sec
Fraction sorbed to airborne particulates (phi):
5.12E-010 (Junge-Pankow, Mackay avg)
4.14E-010 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation




KOCWIN Program (v2.00) Results:
==============================
SMILES : C(=C)CL
CHEM  : Ethene, chloro-
MOL FOR: C2 H3 CL1
MOL WT : 62.50
--------------------------- KOCWIN v2.01 Results ---------------------------

Koc Estimate from MCI:
```

```
---------------------
First Order Molecular Connectivity Index ........... : 1.414
Non-Corrected Log Koc (0.5213 MCI + 0.60) .......... : 1.3370
Fragment Correction(s) --> NONE            :  ---
Corrected Log Koc .................................. : 1.3370

Estimated Koc: 21.73 L/kg  <===========

Koc Estimate from Log Kow:
-------------------------
Log Kow (User entered  ) ......................... : 1.38
Non-Corrected Log Koc (0.8679 logKow - 0.0004) ..... : 1.1973
Fragment Correction(s) --> NONE            :  ---
Corrected Log Koc .................................. : 1.1973

Estimated Koc: 15.75 L/kg  <===========




HYDROWIN Program (v2.00) Results:
================================
SMILES : C(=C)CL
CHEM  : Ethene, chloro-
MOL FOR: C2 H3 CL1
MOL WT : 62.50
--------------------------- HYDROWIN v2.00 Results ---------------------------


Currently, this program can NOT estimate a hydrolysis rate constant for
the type of chemical structure entered!!

ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens),
Specific Alkyl Halides & Phosphorus Esters can be estimated!!

When present, various hydrolyzable compound-types will be identified.
For more information, (Click OVERVIEW in Help or see the User's Guide)

*****  CALCULATION NOT PERFORMED  *****



BCFBAF Program (v3.01) Results:
==============================
SMILES : C(=C)CL
CHEM  : Ethene, chloro-
MOL FOR: C2 H3 CL1
MOL WT : 62.50
--------------------------------- BCFBAF v3.01 --------------------------------
Summary Results:
Log BCF (regression-based estimate): 0.58 (BCF = 3.78 L/kg wet-wt)
Biotransformation Half-Life (days) : 0.242 (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic): 0.50 (BAF = 3.17 L/kg wet-wt)

Log Kow (experimental): 1.46
Log Kow used by BCF estimates: 1.38 (user entered)

Equation Used to Make BCF estimate:
Log BCF = 0.6598 log Kow - 0.333 + Correction

```

```
Correction(s):          Value
No Applicable Correction Factors

Estimated Log BCF = 0.578 (BCF = 3.78 L/kg wet-wt)

===========================================================
Whole Body Primary Biotransformation Rate Estimate for Fish:
===========================================================
------+-----+--------------------------------------------+---------+---------
TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION | COEFF | VALUE
------+-----+--------------------------------------------+---------+---------
Frag | 1 | Aliphatic chloride  [-CL]          | 0.3608 | 0.3608
Frag | 3 | -C=CH [alkenyl hydrogen]           | 0.0988 | 0.2965
Frag | 3 | -C=CH [alkenyl hydrogen]           | 0.0000 | 0.0000
L Kow| * | Log Kow =  1.38 (user-entered  )      | 0.3073 | 0.4241
MolWt| * | Molecular Weight Parameter          |      | -0.1603
Const| * | Equation Constant               |      | -1.5371
============+============================================+=========+=========
RESULT  |    LOG Bio Half-Life (days)       |      | -0.6159
RESULT  |      Bio Half-Life (days)       |      | 0.2422
NOTE   | Bio Half-Life Normalized to 10 g fish at 15 deg C  |
============+============================================+=========+=========

Biotransformation Rate Constant:
kM (Rate Constant): 2.862 /day (10 gram fish)
kM (Rate Constant): 1.61 /day (100 gram fish)
kM (Rate Constant): 0.9052 /day (1 kg fish)
kM (Rate Constant): 0.509 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
Estimated Log BCF (upper trophic) = 0.501 (BCF = 3.168 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 0.501 (BAF = 3.168 L/kg wet-wt)
Estimated Log BCF (mid trophic)   = 0.395 (BCF = 2.482 L/kg wet-wt)
Estimated Log BAF (mid trophic)   = 0.395 (BAF = 2.482 L/kg wet-wt)
Estimated Log BCF (lower trophic) = 0.364 (BCF = 2.31 L/kg wet-wt)
Estimated Log BAF (lower trophic) = 0.364 (BAF = 2.31 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) = 0.539 (BCF = 3.459 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 0.544 (BAF = 3.499 L/kg wet-wt)





Volatilization From Water
=========================

Chemical Name: Ethene, chloro-

Molecular Weight  : 62.50 g/mole
Water Solubility  : 9150 ppm
Vapor Pressure    : 2550 mm Hg
Henry's Law Constant: 0.0278 atm-m3/mole (entered by user)

RIVER       LAKE
---------     ---------
Water Depth    (meters):  1         1
Wind Velocity   (m/sec):  5         0.5
Current Velocity (m/sec):  1         0.05
```

```

HALF-LIFE (min ) :  49.4       4516
HALF-LIFE (hours) :  0.8234      75.27
HALF-LIFE (days ) :  0.03431      3.136


STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
=====================================================================
(using 10000 hr Bio P,A,S)
PROPERTIES OF: Ethene, chloro-
-------------
Molecular weight (g/mol)                62.5
Aqueous solubility (mg/l)               9150
Vapour pressure (Pa)                  339972
(atm)                3.35526
(mm Hg)               2550
Henry 's law constant (Atm-m3/mol)           0.0278
Air-water partition coefficient           1.13694
Octanol-water partition coefficient (Kow)       23.9883
Log Kow                         1.38
Biomass to water partition coefficient         5.59767
Temperature [deg C]                  25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):
-Primary tank    0.01    110.71    10000.00
-Aeration tank    0.01    110.71    10000.00
-Settling tank    0.01    110.71    10000.00

STP Overall Chemical Mass Balance:
---------------------------------
g/h        mol/h     percent

Influent          1.00E+001     1.6E-001    100.00

Primary sludge       3.03E-002     4.8E-004     0.30
Waste sludge        1.33E-002     2.1E-004     0.13
Primary volatilization   1.30E-001     2.1E-003     1.30
Settling volatilization   3.10E-002     5.0E-004     0.31
Aeration off gas      8.95E+000     1.4E-001    89.46

Primary biodegradation   1.75E-003     2.8E-005     0.02
Settling biodegradation   4.58E-005     7.3E-007     0.00
Aeration biodegradation   6.15E-004     9.8E-006     0.01

Final water effluent    8.46E-001     1.4E-002     8.46

Total removal        9.15E+000     1.5E-001    91.54
Total biodegradation    2.41E-003     3.9E-005     0.02
```