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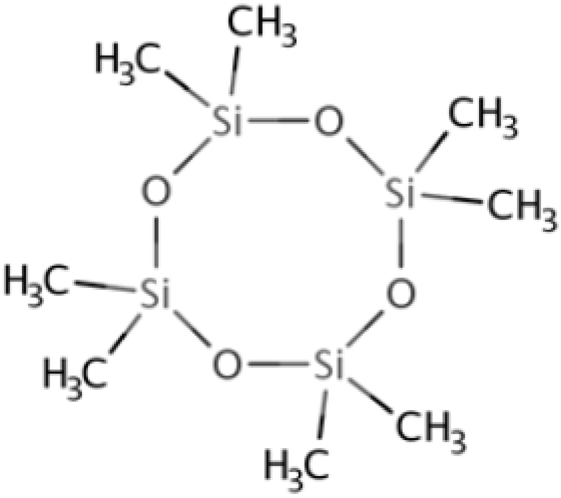
Draft Physical Chemistry and Fate Assessment for Octamethylcyclotetrasiloxane (D4)

Technical Support Document for the Draft Risk Evaluation

CASRN 556-67-2



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ABBREVIATIONS AND ACRONYMS

BAF	Bioaccumulation factor
BCF	Bioconcentration factor
BCF_k	Kinetic bioconcentration factor
BCF_{ss}	Steady-state bioconcentration factor
BMF	Biomagnification factor
BMF_k	Kinetic biomagnification factor

BMF_{ss}	Steady-state biomagnification factor
BMF_{L}	Lipid-normalized biomagnification factor
BSAF	Biota-sediment accumulation factor
CASRN	Chemical Abstracts Service Registry Number
CFR	Code of Federal Regulations
CTD	Characteristic travel distance
D4	Octamethylcyclotetrasiloxane
D5	Decamethylcyclopentasiloxane
D6	Dodecamethylcyclohexasiloxane
DMR	Discharge Monitoring Report
DMSD	Dimethylsilanediol
DOC	Dissolved organic carbon
dw	Dry weight
ECA	Enforceable Consent Agreement
EPA	Environmental Protection Agency (U.S.)
EPI Suite™	Estimation Program Interface Suite™ (model)
FR	Federal Register
K_{AW}	Air/water partition coefficient
K_{DOC}	Dissolved organic carbon/water partition coefficient
K_{OA}	Octanol/air partition coefficient
K_{OC}	Organic carbon/water partition coefficient
K_{OW}	Octanol/water partition coefficient
K_{SW}	Soil/water partition coefficient
LRTP	Long-range transport potential
MDL	Method detection limit
n.d.	Not-detects
OC	Organic carbon
OECD	Organisation for Economic Co-operation and Development
•OH	Hydroxyl radical
PDMS	Polydimethylsiloxane
P_{OV}	Overall persistence
SE	Standard error of the mean
STP	Sewage treatment plant
$t_{1/2}$	Half-life
TE	Transfer efficiency
TG	Test guideline
TMF	Trophic magnification factor
TRI	Toxics Release Inventory
U.S.	United States
ww	Wet weight
WWTP	Wastewater treatment plant

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Docket

Supporting information can be found in the public docket, Docket ID EPA-HQ-OPPT-2018-0443.

Disclaimer

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SUMMARY

This technical support document is in support of the TSCA *Draft Risk Evaluation for Octamethylcyclotetrasiloxane (D4)* (U.S. EPA, 2025b). EPA gathered and evaluated the reasonably available information to characterize the physical and chemical properties as well as environmental fate and transport of D4. The key points are summarized below:

- D4 is found in various environmental media including air, water, sediment, soil and biota due to its widespread production and application.
- The physical and chemical properties of D4 determine its environmental fate and transport behavior, which is important in understanding D4's persistence in the environment and its potential for bioaccumulation, while considering transport, partitioning, and removal pathways. D4 is a smooth, viscous liquid that is hydrophobic and volatile. Based on D4's water solubility (0.056 mg/L 23 °C), Henry's law constant (11.8 atm·m^3/mol at 21.7 °C), and log K_{OC} values (4.19–4.22 at 24.4–24.8 °C), D4 will preferentially partition to organic carbon, which suggests that the major environmental compartments will be air, soil, biosolids, and sediment.
- D4 is expected to undergo rapid hydrolysis in aquatic environments with dimethylsilanediol (DMSD) as its final product. However, D4's hydrolysis rate is highly dependent on pH and temperature. In addition, D4 is not expected to undergo photolysis in aquatic environments under environmentally relevant conditions since it does not absorb wavelengths greater than 290 nm.
- D4 does not undergo biodegradation in water under aerobic conditions. In most natural surface water (pH 6–8), volatilization will be the dominant process for D4 due to its vapor pressure (0.9338 mm Hg at 25 °C) and Henry's law constant (11.8 atm·m^3/mol at 21.7 °C). Hydrolysis of D4 under neutral conditions will be much slower. In alkaline waters ($pH \geq 9$), hydrolysis will be the dominant mechanism but volatilization will still occur first.
- D4 is not expected to undergo significant direct photolysis and D4 in the gaseous phase is expected to degrade slowly by reaction with photochemically produced hydroxyl radicals (•OH) in the atmosphere ($t_{1/2}$ = 4.7–11.4 days). D4 has the potential to undergo atmospheric long-range transport due to its persistence in the atmosphere.
- D4 can be transported to sediments from overlying surface water via advection, dispersion, and sorption to suspended solids that can settle out from the water column. D4 does not undergo biodegradation in sediment under aerobic and anaerobic conditions. Due to its log K_{OC} (4.19–4.22 at 24.4–24.8 °C) and log K_{OW} (6.488 at 25.1 °C) values, D4 will have a strong affinity for organic carbon in sediment.
- D4 is not expected to be mobile and will adsorb strongly to organic matter in soil based on its log K_{OC} values (4.19–4.22 at 24.4–24.8 °C) and water solubility (0.056 mg/L at 23 °C). Also, D4 is likely to volatilize from moist soil due to its high volatility and log K_{AW} (2.69 at 21.7 °C) and hydrolyze in soil with higher acidity and clay content.
- D4 disposed to municipal solid waste incineration will be effectively degraded (>99.9%) and its emission through incineration ash landfill will be negligible. Incineration plants are not expected to be significant sources of D4 releases to the air.
- The removal of D4 in wastewater treatment will be primarily by sorption to sludge and volatilization. Biodegradation is not expected to be a significant removal process. The remaining small fraction of D4 in the wastewater effluent may be discharged to receiving water. D4 removed by sorption to sewage sludge may be transferred to soil through biosolids amendment.
- D4 is highly likely to bioconcentrate and bioaccumulate in fish (mean BCF = 8,795 L/kg), and may accumulate in sediment-dwelling organisms.

- While field-derived BMF values greater than one have been reported for specific predator-prey relationships, overall D4 is unlikely to biomagnify. Also, D4 is not expected to exhibit trophic magnification.
- Overall, D4 meets the criteria for both a 'Persistent' and 'Very Persistent' substance in air and sediment under the EPA New Chemicals framework (64 FR 60194, November 4, 1999). D4 also meets the criteria for both a 'Bioaccumulative' and 'Very Bioaccumulative' substance in biota. However, D4 is not expected to be persistent in water and soil under environmentally relevant conditions but may be persistent in water where there is continuous release of D4.

1 INTRODUCTION

Octamethylcyclotetrasiloxane (D4) belongs to a group of cyclic volatile methylsiloxanes (cVMS) that consist of cyclic chains of alternating silicon (Si) and oxygen (O) atoms with methyl groups (CH_3) $[–Si(CH_3)_2–O–]_x$ and D4 consists of four of these chains (x = 4) (Chandra, 1997; EC/HC, 2008c; Brooke et al., 2009c; Panagopoulos and Macleod, 2018). D4 is manufactured by several sequential reactions that include: 1) the reduction of quartz to silicon (Si); 2) reaction of silicon metal with methyl chloride (CH_3Cl) to produce chlorosilanes; 3) the hydrolysis of chlorosilanes; 4) and the condensation of short chain chlorosilanes to siloxanes (SEHSC, 2020).

Due to its unique physical and chemical properties, D4 is primarily used as an intermediate in the manufacture of other silicone chemicals such as polydimethylsiloxane (PDMS) and as an ingredient in commercial and consumer products, including sealants, adhesives, and cleaning, laundry, and dishwashing products (Wang et al., 2001; EC/HC, 2008c; Horii and Kannan, 2008; Brooke et al., 2009c; Cheng et al., 2011; Fromme et al., 2019; NICNAS, 2020). Because D4 is used in a wide range of applications, it is found in various environmental media including air (Section 3.4.1), water (Section 3.4.2.1), sediment (Section 3.4.2.2), soil (Section 3.4.3.2), and biota (Section 3.6).

2 PHYSICAL AND CHEMISTRY ASSESSMENT

2.1 Approach and Methodology

EPA gathered and evaluated physical and chemical property data and information according to the process described in the *Draft Systematic Review Protocol Supporting TSCA Risk Evaluations for Chemical Substances* (U.S. EPA, 2021d) (also referred to as the "2021 Draft Systematic Review Protocol"). During the evaluation of D4, EPA considered both measured and estimated physical and chemical property data/information. EPA selected empirical and measured data over modeled data as much as possible to improve the confidence in the endpoints. Due to the relative availability of data, only studies with an overall quality data determination of "High" were selected for use in determining the representative physical and chemical properties of D4 for the purposes of the draft risk evaluation.

A composite plot consisting of box and whisker plots of reported high- and medium-quality physical and chemical property data values is shown in Figure 2-1. 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 selected for use in this risk evaluation is overlaid (indicated by the orange star) to provide context for where it lies within the distribution of the data set. Information on the full, extracted dataset is available in the supplemental file, *Draft Data Quality Evaluation and Data Extraction Information for Physical and Chemical Properties of Octamethylcyclotetrasiloxane (D4)* (U.S. EPA, 2025d).

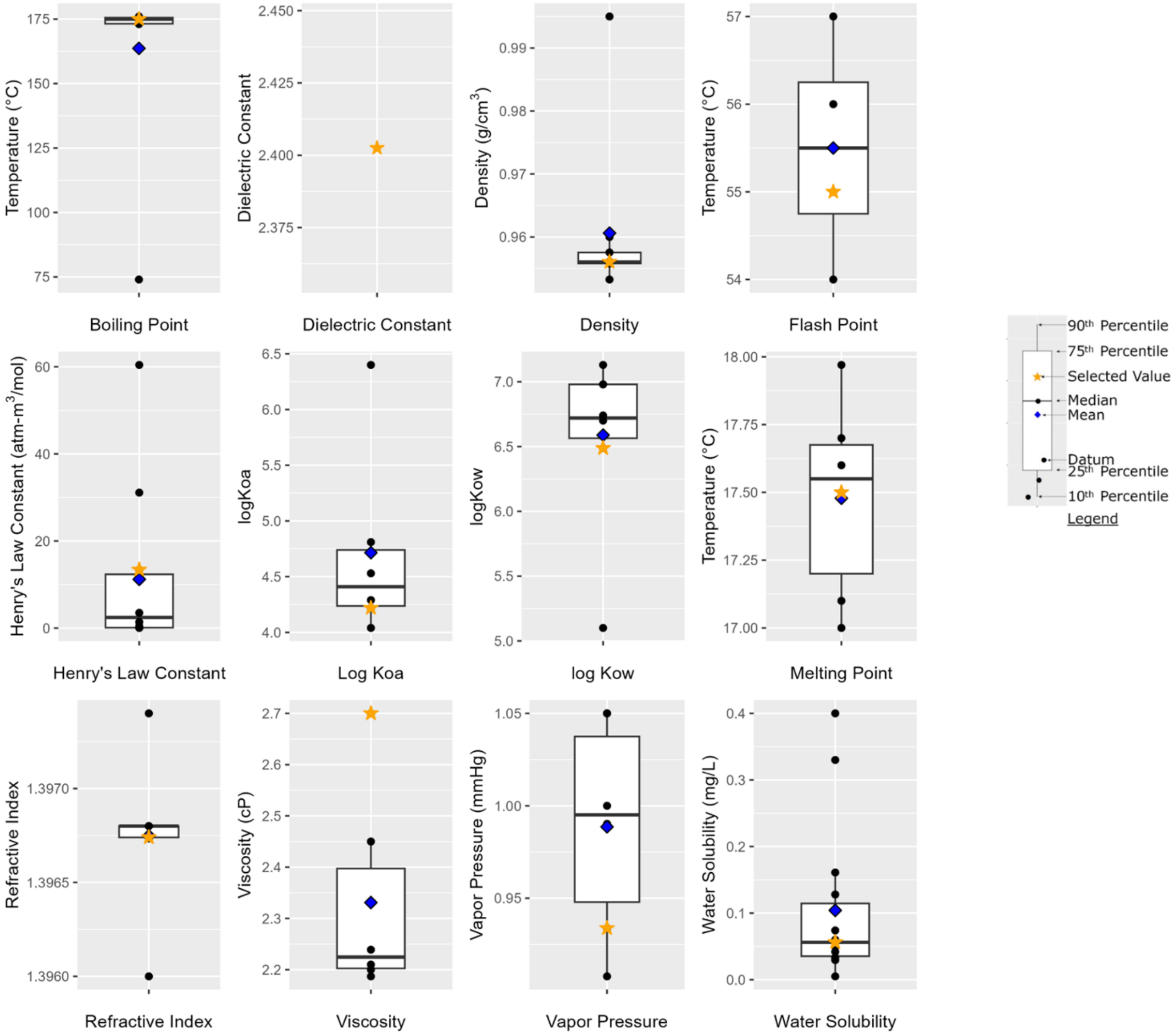

Figure 2-1. Box and Whisker Plots of Reported Physical and Chemical Property Data Values

D4 undergoes abiotic ring opening in water, soil, and sediment to form octamethyltetrasiloxanediol (tetramer diol; CASRN 3081-07-0), which subsequently undergoes step-wise abiotic degradation through hexamethyltrisiloxanediol (trimer diol; CASRN 3663-50-1) and tetramethyldisiloxanediol (dimer diol; CASRN 1118-15-6) into the stable end-product dimethylsilanediol (DMSD) (CASRN 1066-42-8) (Figure 2-2) (Xu and Chandra, 1999; Durham, 2005; Xu and Miller, 2008). Studies have reported that DMSD aerobically biodegrades in soil into silicic acid (H_4O_4Si; CASRN 10193-36-9) under specific field and laboratory conditions (Sabourin et al., 1996; Lehmann et al., 1998; Sabourin et al., 1999). Silicic acid was not considered since it is a naturally occurring small molecule from the weathering of rocks or diatoms, which exists independently from siloxanes. Based on this, EPA extracted and evaluated physical and chemical property values for the degradants, except silicic acid, and are presented in Table 2-2. The rationale for each selected value is provided in Appendix A.1.3. The references and data quality ratings for each selected value are provided in Table_Apx A-1, Table_Apx A-2, Table_Apx A-3, and Table_Apx A-4.

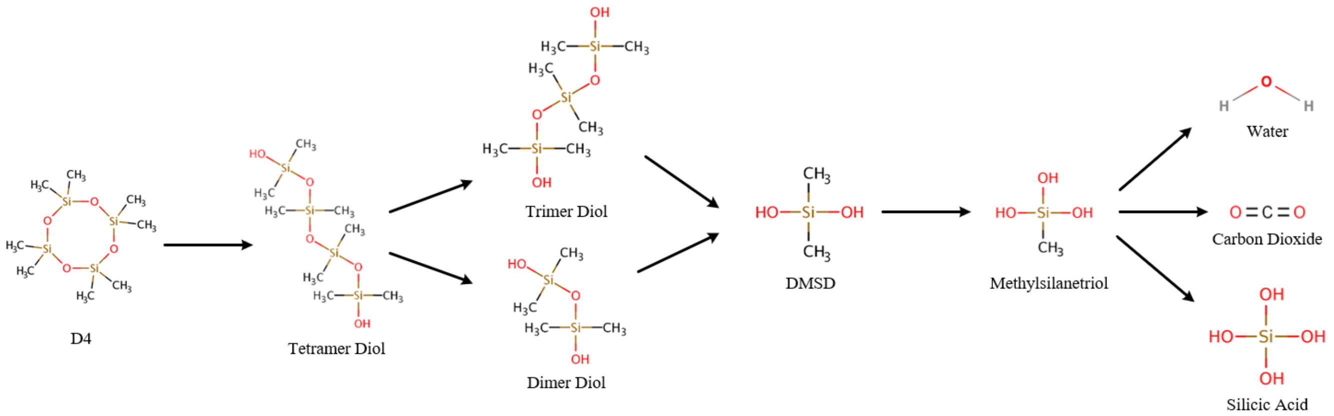

Figure 2-2. Summary of a Complete D4 Mineralization

2.2 Final Selected Physical and Chemical Property Values

The physical and chemical property values selected for use in this risk evaluation for D4 are given in Table 2-1. For some physical and chemical properties, there are multiple high-quality values available for selection that were identified during systematic review. The majority of selected data were collected under standard environmental conditions (*i.e.*, 20–25 °C and 760 mm Hg). However, some properties are reported at several experimental temperatures to provide additional context to how D4 behaves under environmentally relevant temperatures in real world scenarios. This is especially important for providing foundational context for environmental fate and transport endpoints (*i.e.*, biodegradation rates, wastewater removal efficiency, bioaccumulation factors, etc.) as they demonstrate the variety of environmental conditions where D4 may be measured.

D4 exists as a smooth, viscous liquid (DOE (2016); NCBI (2021) citing Lewis and Hawley (2007) and O'Neil (2013)). D4 has a melting point of 17.5 °C (O'Neil, 2013; DOE, 2016; RSC, 2020; NCBI, 2021) and a boiling point of 175 °C (O'Neil, 2013; Haynes, 2014b; DOE, 2016; NCBI, 2021). D4 has a vapor pressure of 0.9338 mm Hg at 25 °C (Lei et al., 2010), a water solubility of 0.056 mg/L at 23 °C (Dow Corning, 1991; Varaprath et al., 1996; NCBI, 2021), and a Henry's law constant of 11.8 atm·m^3/mol at 21.7 °C (Xu and Kropscott, 2012, 2014; NCBI, 2021).

Table 2-1. Physical and Chemical Properties of D4

Property	Selected Value(s)[a]	Reference(s)	Data Quality Rating[b]
Molecular formula	$C_8H_{24}O_4Si_4$	NCBI (2021)	High
Molecular weight	296.61 g/mol	Haynes (2014b)	High
Physical form	Smooth, viscous liquid	Lewis and Hawley (2007) and O'Neil (2013) as cited in DOE (2016) and NCBI (2021)	High
Melting point	17.5 °C	O'Neil (2013); DOE (2016); RSC (2020); NCBI (2021)	High
Boiling point	175 °C	O'Neil (2013) as cited in Haynes (2014b), DOE (2016), and NCBI (2021)	High
Density	0.95603 g/cm^3 at 20 °C	Zhang et al. (2015)	High
Vapor pressure	0.9338 mm Hg at 25 °C	Lei et al. (2010)	High

Vapor density	No data identified		
Water solubility	0.056 mg/L at 23 °C	Dow Corning (1991), Dow Corning (1993b), and Varaprath et al. (1996) as cited in NCBI (2021)	High
Octanol/water partition coefficient (log K_{OW})	6.488 ± 0.017 at 25.1 °C (OECD 123)	Kozerski and Shawl (2007)	High
	6.59 ± 0.07 at 5.7 °C 6.98 ± 0.13 at 21.7 °C 7.13 ± 0.1 at 34.8 °C	Xu and Kropscott (2012); Xu and Kropscott (2014)	
Octanol/air partition coefficient (log K_{OA})	4.29 ± 0.03 at 21.7 °C 4.22 ± 0.01 at 24 °C	Xu (2006), Xu and Kropscott (2007), and Xu and Kropscott (2012) as cited in SEHSC (2020)	High
	4.81 ± 0.02 at 5.7 °C 4.53 ± 0.08 at 12.2 °C 4.04 ± 0.07 at 34.8 °C	Xu and Kropscott (2014)	
Henry's law constant	1.4 atm·m^3/mol at 5.7 °C 3.5 atm·m^3/mol at 12.2 °C 11.8 atm·m^3/mol at 21.7 °C 31.1 atm·m^3/mol at 34.8 °C	Xu and Kropscott (2012); Xu and Kropscott (2014)	High
Flash point	55 °C (closed cup)	Sigma Aldrich (2020) as cited in NCBI (2021)	High
Autoflammability	No data identified		
Viscosity	2.45 cP at 20 °C	Palczewska-Tulinska and Oracz (2005)	High
	2.7 cP at 26.95 °C	Liu et al. (2013)	
Refractive index	1.39674 at 20 °C	Zhang et al. (2015)	High
Dielectric constant	2.4–2.405 at 20 °C	Elsevier (2019)	High

[a] Measured unless otherwise noted
[b] "Data Quality Rating" apply to all references listed in this table

Table 2-2. Physical and Chemical Properties of D4 Degradants

Property	DMSD	Dimer Diol	Trimer Diol	Tetramer Diol
Molecular formula	$C_2H_8O_2Si$	$C_4H_{14}O_3Si_2$	$C_6H_{20}O_4Si_3$	$C_8H_{26}O_5Si_4$
CASRN	1066-42-8	1118-15-6	3663-50-1	3081-07-0
Molecular weight	92.17 g/mol	166.33 g/mol	240.48 g/mol	314.64 g/mol
Physical form	Crystal phase – interplanar spacing and leafs	Needle-shaped, monoclinic, white crystal	No data identified	No data identified
Melting point	94.5–101 °C	66 °C	–23 to –1.9 °C	–5 °C
Boiling point	No data identified	No data identified	79–91 °C	86–88 at 0.4 torr 97–100 at 2 torr
Density	1.095–1.099 g/cm^3	1.095 g/cm^3 at 25 °C	0.991–1.0127 g/cm^3 at 20–25 °C	0.9881–0.9886 g/cm^3 at 20 °C
Vapor pressure	No data identified	No data identified	No data identified	No data identified
Vapor density	No data identified	No data identified	No data identified	No data identified
Water solubility	2.45E06 mg/L at 25 °C	110,000–115,000 mg/L at 20–25 °C	No data identified	No data identified
Octanol/water partition coefficient (log K_{OW})	–0.41 ± 0.1 at 20.1 °C	0.926 ± 0.035 at 12 °C 0.962 ± 0.049 at 20 °C 1.036 ± 0.042 at 27 °C 1.099 ± 0.025 at 35 °C	2.125 ± 0.249 at 12 °C 2.369 ± 0.104 at 20 °C 2.391 ± 0.112 at 27 °C 2.512 ± 0.165 at 35 °C	No data identified
Octanol/air partition coefficient (log K_{OA})	6.40 ± 0.31 at 20.1 °C	No data identified	No data identified	No data identified
Henry’s law constant	3.48E–09 atm·m^3/mol at 20.1 °C	2.58E–07 atm·m^3/mol at 12 °C 5.25E–07 atm·m^3/mol at 20 °C 1.73E–07 atm·m^3/mol at 27 °C 1.39E–07 atm·m^3/mol at 35 °C	1.12E–06 atm·m^3/mol at 12 °C 1.23E–06 atm·m^3/mol at 20 °C 1.13E–06 atm·m^3/mol at 27 °C 1.37E–06 atm·m^3/mol at 35 °C	No data identified
Flash point	No data identified	No data identified	No data identified	No data identified
Autoflammability	No data identified	No data identified	No data identified	No data identified
Viscosity	No data identified	No data identified	No data identified	No data identified
Refractive index	1.444–1.456 at 25 °C	1.457–1.466 at 25 °C	1.405–1.409 at 20–25 °C	1.4054–1.4088 at 20–25 °C

2.3 Endpoint Assessments

The physical and chemical property values were taken from the *Final Scope of the Risk Evaluation for Octamethylcyclotetrasiloxane (Cyclotetrasiloxane, 2,2,4,4,6,6,8,8-octamethyl-) (D4); CASRN 556-67-2* (U.S. EPA, 2022b) (hereinafter referred to as the "final scope") except for vapor pressure, octanol/water partition coefficient (log K_{OW}), octanol/air partition coefficient (log K_{OA}), Henry's law constant, and viscosity, which were updated based on systematic review results added since the publication of the final scope.

2.3.1 Vapor Pressure

A vapor pressure of 1.05 mm Hg at 25 °C from NCBI (2021) was reported in the final scope for D4 (U.S. EPA, 2022b). Six high- and three medium-quality vapor pressure data were extracted and evaluated through systematic review after the publication of the final scope. Three medium-quality vapor pressure data were excluded for use in this risk evaluation because high-quality vapor pressure data are available. The high-quality data from NIST (2022) was excluded for use in this risk evaluation because a vapor pressure was reported without an experimental temperature and the other three vapor pressures were measured at higher temperature ranges (≥102.9 °C). Due to this, there is insufficient evidence that these data are representative of D4 behavior under standard environmental conditions. The vapor pressure data from NCBI (2021), U.S. EPA (2020), and Kochetkov (2001) were also excluded for use in this risk evaluation because they were modeled data. The vapor pressure of 0.9338 mm Hg at 25 °C from Lei (2010) was selected for use in this risk evaluation because it was obtained from an acceptable laboratory study and had the highest metric score (U.S. EPA, 2021d).

2.3.2 Octanol/Water Partition Coefficient (log K_{OW})

The log K_{OW} values of 6.59 ± 0.07, 6.98 ± 0.13, and 7.13 ± 0.1 at 5.7, 21.7, and 34.8 °C, respectively, (Xu and Kropscott, 2012, 2014) were reported in the final scope for D4 (U.S. EPA, 2022b). These high-quality data were collected using a double-syringe apparatus that allowed for the concurrent determination of internally consistent K_{OW}, K_{OA}, and K_{AW} partitioning coefficients with precision (Xu and Kropscott, 2012, 2014). After the final scope was published, eight high-quality log K_{OW} data for D4 were extracted and evaluated during systematic review. Three data points were excluded because no experimental temperature was reported (Dow Corning, 1982, 1987; U.S. EPA, 2020). NCBI (2021) reported a log K_{OW} value of 6.74 at 25 °C, which was an average of three measurements from Xu et al. (2014). However, the study reported log K_{OW} values of 6.49, 4.45, and 6.98 at 25 °C, resulting in an average of 5.97. Xu et al. (2014) also reported a log K_{OW} value of 6.98 at 22 °C. When including the fourth reported log K_{OW} value, it gives a mean log K_{OW} value of 6.225. Due to uncertainty in the source of this error, the log K_{OW} of 6.74 data point was excluded from consideration. Kozerski et al. (2007) reported a log K_{OW} value of 6.488 ± 0.017 at 25.1 °C using the slow-stirring method as described in OECD Test Guideline (TG) 123 (OECD, 2022b). The high-quality data published by Kozerski et al. (2007), Xu and Kropscott (2012), and Xu et al. (2014) were selected for use in this risk evaluation.

2.3.3 Octanol/Air Partition Coefficient (log K_{OA})

No log K_{OA} data were reported in the final scope for D4 (U.S. EPA, 2022b). After the final scope was published, three high-quality and one medium-quality log K_{OA} data were extracted and evaluated in the systematic review process. The medium-quality data (Compton, 2019) was excluded from use in this risk evaluation. SEHSC (2020) reported high-quality log K_{OA} data from two different studies: 4.22 ± 0.03 at 24 °C (Xu, 2006) and 4.29 ± 0.03 at 21.7 °C (Xu and Kropscott, 2007, 2012). Xu and Kropscott (2014) reported high-quality log K_{OA} values of 4.81 ± 0.02, 4.53 ± 0.08, and 4.04 ± 0.07 at 5.7, 12.2, and 34.8 °C, respectively. Xu and Kropscott (2012) reported log K_{OA} values of 4.28 ± 0.04 at 21.7 °C and 4.30 ± 0.02 at 21.6 °C, which brings to a mean log K_{OA} value of 4.29 ± 0.03 at 21.7 °C. All of the above-listed, high-quality log K_{OA} data were selected for use in this risk evaluation ((Xu and Kropscott, 2012, 2014) as cited in (SEHSC, 2020)).

2.3.4 Henry's Law Constant

Henry's law constant values of 1.4, 11.8, and 31.1 atm·m^3/mol at 5.7, 21.7, and 34.8 °C, respectively (Xu and Kropscott, 2012, 2014) were reported in the final scope for D4 (U.S. EPA, 2022b). After the final scope was published, nine air/water partition coefficient (K_{AW}) data for D4 were extracted and evaluated during systematic review. Henry's law constant is in direct relation with K_{AW} (Mackay et al., 2006) and can be determined by using Equation 2-1.

Equation 2-1

$$HLC = R \times T \times K_{AW}$$

Where:

HLC = Henry's law constant (atm·m^3/mol)
R = Universal gas constant (8.206×10^{-5} atm·m^3/mol·K)
T = Temperature (K)
K_{AW} = Dimensionless air/water partition coefficient

An uninformative study, Kochetkov et al. (2001), was excluded from this risk evaluation because the reporting of the study was inconsistent. Different values for the same measurements were reported throughout the study. Two high-quality studies were also excluded from this risk evaluation because no experimental temperature was reported (NCBI (2021), citing U.S. EPA (2020) and U.S. EPA (2021c)). The data from Ann Arbor Technical Services (1990) and Ann Arbor Technical Services (2000) had low measurement precision (log scale standard deviations ≥ 0.84), decreasing confidence in the reported log K_{AW}. In addition, Ann Arbor Technical Services (1990) was unable to confirm equilibrium conditions when taking air and water measurements, and its data are therefore considered unreliable. For these reasons, the data from Ann Arbor Technical Services (1990, 2000) were excluded from this risk evaluation. A log K_{AW} value of 2.74 at 25 °C was interpolated by Xu and Kropscott (2014) using the linear regression of log K_{AW} values on the reciprocal of equilibrium temperature (T) in Kelvin. This is equivalent to a Henry's law constant of 13.4 atm·m^3/mol (NCBI, 2021). This data was not selected for use in this risk evaluation because high-quality empirical log K_{AW} values are available.

Hamelink et al. (1996) reported a mean undimensioned Henry's law constant value of 3.4 ± 1.37 at 20 °C, which is equivalent to a Henry's law constant value of 0.0819 atm·m^3/mol. D4 measurements were obtained using the purge and trap technique, and sampled at periods of 24, 48, 72, and 96 hours. Henry's law constant was seen to increase from 1 to 72 hours, then decreased from 72 to 120 hours over the course of the experiment. It was concluded that equilibrium was not confirmed in this experiment, therefore it was excluded from this risk evaluation.

Xu and Kropscott (2014) also reported a log K_{AW} value of 2.17 ± 0.08 at 12.2 °C, which is equivalent to 3.5 atm·m^3/mol and is selected for use in this risk evaluation. The measured mean log K_{AW} value of 2.69 at 21.7 °C (Xu and Kropscott, 2012) is in good agreement with the log K_{AW} temperature dependence yielded by the above-listed measurements by Xu and Kropscott. (2014). The reported log K_{AW} value of 2.69 at 21.7 °C (Xu and Kropscott, 2014) is in good agreement with the equilibrium of the three measured partition coefficients (Equation 2-2).

Equation 2-2

$$Log\ K_{OW} = Log\ K_{OA} + Log\ K_{AW}$$

Where:

$Log\ K_{OW}$ = Logarithmic octanol/water partition coefficient
$Log\ K_{OA}$ = Logarithmic octanol/air partition coefficient
$Log\ K_{AW}$ = Logarithmic air/water partition coefficient

2.3.5 Viscosity

A viscosity value of 2.30 centipoise (cP) at 25 °C (NCBI, 2021) was reported in the final scope (U.S. EPA, 2022b), but the viscosity unit was incorrectly reported. NCBI (2021) reported a viscosity of 2.30 centistokes (cSt) at 25 °C. In order to convert it to the cP unit, Equation 2-3 is used.

Equation 2-3

$$\eta = \nu \times \rho$$

Where:

η = dynamic viscosity
ν = kinematic viscosity (2.30 cSt)
ρ = density (0.96 g/cm^3)

This would give us a viscosity of 2.21 cP at 25 °C. However, this datum was excluded because the original study could not be located, so the laboratory method could not be verified. For this risk evaluation, both 2.45 cP at 20 °C (Palczewska-Tulinska and Oracz, 2005) and 2.7 cP at 26.95 °C (Liu et al., 2013) were selected because the data were obtained from laboratory studies and had the highest metric scores.

2.4 Strengths, Limitations, Assumptions, and Key Sources of Uncertainty for the Physical and Chemistry Assessment

The physical and chemical property data discussed in this document were the product of a systematic review of reasonably available information. The data analyses, therefore, 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 dataset. This duplication should be considered as a potential source of uncertainty in the data analyses. However, data-collection procedures and expert judgment were used to minimize this possibility whenever possible.

Due to D4's low water solubility and surface tension, and volatility, certain physical and chemical properties may be difficult to measure experimentally, such as water solubility and partitioning coefficients (*e.g.*, K_{OW}, K_{OA}, K_{AW}) with standard guideline tests. Sometimes those tests can exhibit poor reproducibility as evidenced by large standard deviations (Varaprath et al., 1996; Xu and Kropscott, 2012; Xu et al., 2014; Xu and Kropscott, 2014). The selection of the physical and chemical properties for use in the current risk evaluation was based on professional judgment which incorporated consideration of the overall data quality ranking of the references from the systematic review process.

3 FATE AND TRANSPORT ASSESSMENT

3.1 Approach and Methodology

Reasonably available environmental fate data—including biotic and abiotic biodegradation rates, removal during wastewater treatment, volatilization from lakes and rivers, and organic carbon/water partition coefficient (log K_{OC})—are the parameters used in the current draft risk evaluation. In assessing the environmental fate and transport of D4, EPA considered the full range of results from data sources that were rated high confidence. Information on the full extracted dataset is available in the supplemental file, *Draft Data Quality Evaluation and Data Extraction Information for Environmental Fate and Transport for Octamethylcyclotetrasiloxane (D4)* (U.S. EPA, 2025c). In addition, EPA also integrated robust monitoring data representing a subset of D4 available in the *D4 Environmental Testing Report* {ERM, 2017, 7340832;, 2017, 7360869}. The report was prepared in accordance with an Enforceable Consent Agreement (ECA) between EPA and five D4 manufacturers, processors, or formulators (Dow Corning Corporation, Evonik Corporation, Momentive Performance Materials USA Inc., Shin-Etsu Silicones of America, Inc., and Wacker Chemical Corporation) (U.S. EPA, 2014). It is hereafter referred to as the ECA. The environmental testing program undertaken by five companies was conducted in accordance with a Study Plan and Quality Assurance Project Plan that EPA reviewed and approved, therefore the quality of data in the ECA is thus high.Other fate estimates were based on modeling results from Estimation Programs Interface (EPI) Suite™ (U.S. EPA, 2017), a predictive tool for physical and chemical properties and environmental fate estimation.[1] Information regarding the model inputs is available in Section 3.1.1.

First, EPA conducted a Tier I analysis to identify the environmental compartments (*i.e.*, water, sediment, biosolids, soil, groundwater, air) of major and minor relevance to the fate and transport of D4. Next, a Tier II analysis was conducted to identify the fate pathways and media most likely to cause exposure from environmental releases. The results of the Tier I and II analyses are discussed in Section 3.2. Next, understanding the transformation behavior of D4 informs which pathways are expected to be dominant or contributing to persistence in different compartments. D4 undergoes different transformation processes, and they are discussed in Section 3.3. Since D4 degrades into DMSD in water, soil, and sediment via different intermediate degradants under various conditions, this assessment also includes the transformation behavior of DMSD in the environment (see Appendix A.2). Lastly, EPA assessed the environmental fate and transport of D4 by considering the full range of results from data sources that were rated high confidence and performed media-specific fate analyses as described in Section 3.4.

3.1.1 EPI Suite™ Model Inputs and Settings

To set up EPI Suite™ for estimating fate properties of D4, the “Search CAS” function was used. Then, 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) (Figure 3-1).

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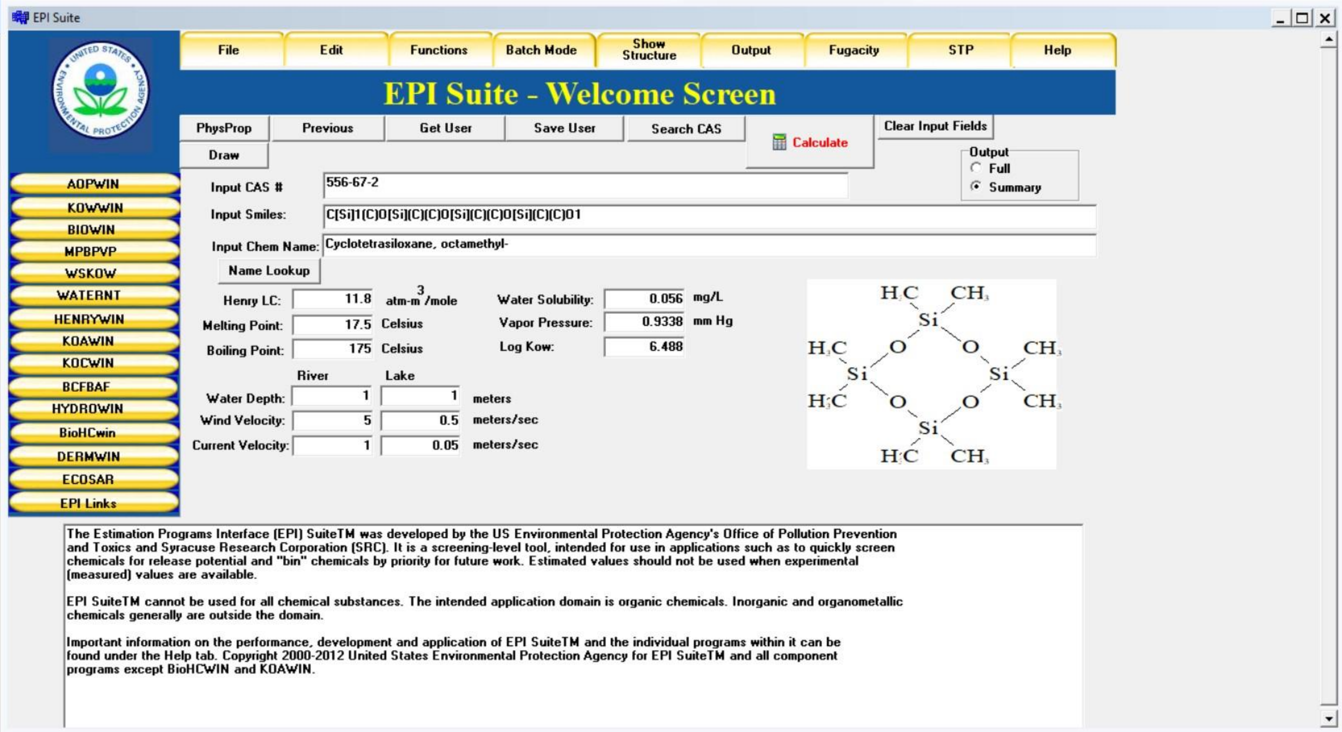
[1] See EPI Suite™ for additional information and supporting documents about this freely available, online suite of programs, which was reviewed by the EPA Science Advisory Board (SAB, 2007).



Output: ○ Full ● Summary

Input CAS #: 556-67-2

Input Smiles: C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1

Input Chem Name: Cyclotetrasiloxane, octamethyl-

Henry LC: 11.8 atm-m^3/mole

Melting Point: 17.5 Celsius

Boiling Point: 175 Celsius

Water Solubility: 0.056 mg/L

Vapor Pressure: 0.9338 mm Hg

Log Kow: 6.488

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

The Estimation Programs Interface (EPI) SuiteTM was developed by the US Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). It is a screening-level tool, intended for use in applications such as to quickly screen chemicals for release potential and "bin" chemicals by priority for future work. Estimated values should not be used when experimental (measured) values are available.

EPI SuiteTM cannot be used for all chemical substances. The intended application domain is organic chemicals. Inorganic and organometallic chemicals generally are outside the domain.

Important information on the performance, development and application of EPI SuiteTM and the individual programs within it can be found under the Help tab. Copyright 2000-2012 United States Environmental Protection Agency for EPI SuiteTM and all component programs except BioHCWIN and KOAWIN.

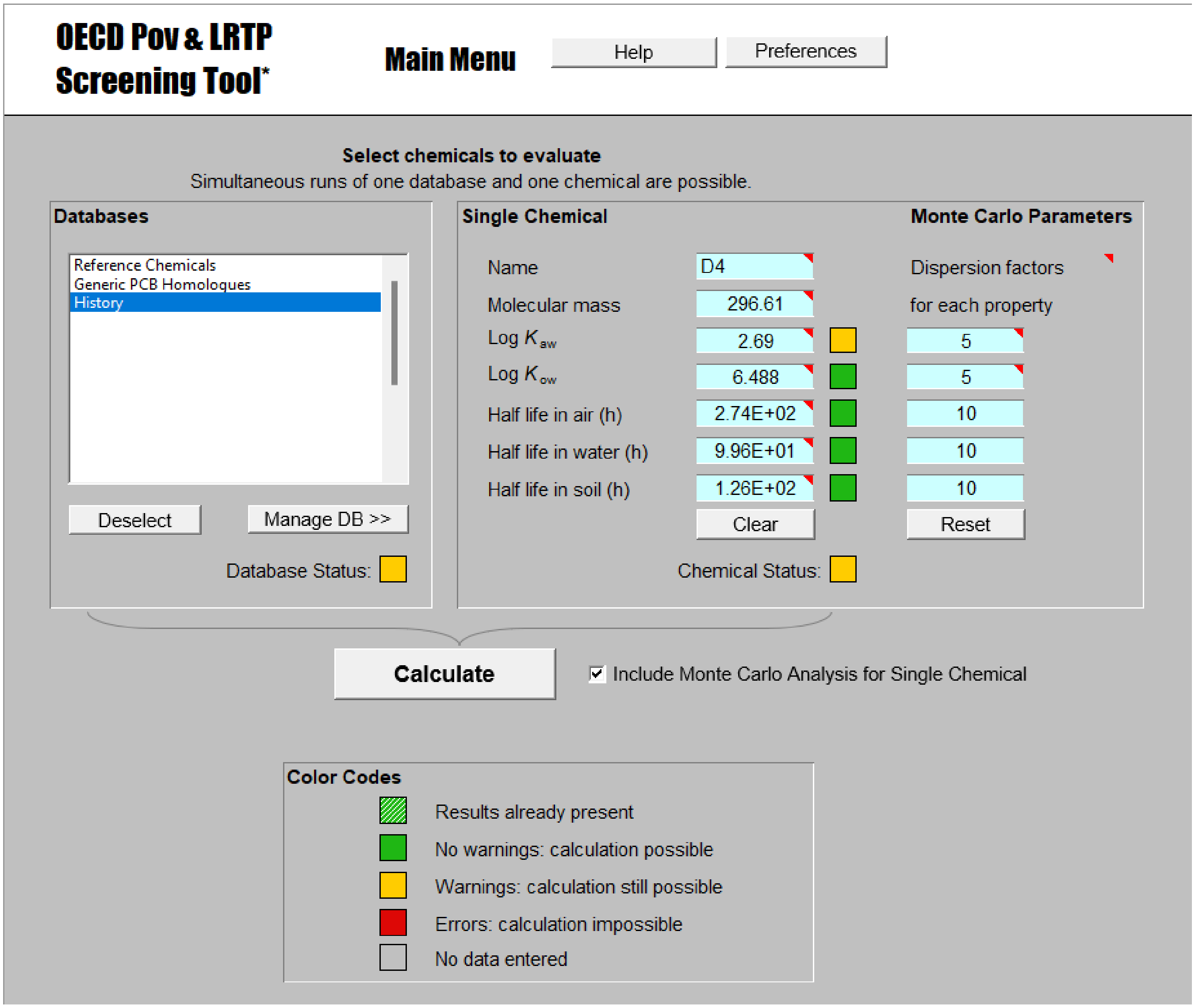
Figure 3-1. Screen Capture of EPI Suite™ Parameters Used to Calculate Physical and Chemical Properties and Environmental Fate for D4

3.1.2 Fugacity Modeling

Fugacity modeling provides an indication of how D4 will be distributed in the environment. The approach described by Mackay et al. (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). D4’s physical and chemical properties were taken directly from Table 2-1. Environmental release information is valuable for fugacity modeling because the emission rates will predict a real-time percent mass distribution for each medium. Due to a lack of data in the Toxics Release Inventory (TRI) and Discharge Monitoring Report (DMR), environmental degradation half-lives were derived from high-quality studies identified through systematic review to reduce the level of uncertainty. The result of the Tier II analysis is discussed in Section 3.2.2.

3.1.3 OECD P_{OV} and LRTP Screening Tool Inputs and Settings

D4’s long-range transport potential (LRTP) was evaluated by using the Organisation for Economic Co-operation and Development (OECD) Overall Environmental Persistence (P_{OV}) and LRTP Screening Tool (Version 2.2) (Wegmann et al., 2009). The OECD P_{OV} and LRTP Tool is a software in a Microsoft Excel spreadsheet format containing multimedia chemical fate models that were designed based on the recommendations of the OECD expert group to estimate environmental persistence and LRTP of organic chemicals at a screening level. With a chemical’s physical and chemical properties, the OECD P_{OV} and LRTP Tool is able to predict its P_{OV}, characteristic travel distance (CTD), and surface transfer efficiency (TE). P_{OV} is the overall persistence in the whole environment in days, CTD quantifies the distance in kilometers (km) from the point of release to the point at which the concentration has dropped to 1/e, or approximately 37 percent of its initial value, and TE estimates the percentage of emitted chemical that is deposited to surface media after transport away from the region of release. The OECD P_{OV} and LRTP Screening Tool calculates two emission scenario-specific CTD values, for emissions to air and water. Only transport in the medium that receives the emission is considered, thus CTD in air is calculated from the emission-to-air scenario and CTD in water is calculated from the emission-to-water scenario. No CTD is calculated for emissions to soil because soil is not considered to be mobile (Wegmann et al., 2009). The physical and chemical properties were input based on the values in Table 2-1, Table 3-1, and Table 3-3 (Figure 3-2). The modeling results are discussed in Sections 3.4.1.1 and 3.4.2.1.



Database Status: 🟨

Single Chemical			Monte Carlo Parameters: Dispersion factors for each property
Name	D4		
Molecular mass	296.61		
Log K_{aw}	2.69	🟨	5
Log K_{ow}	6.488	🟩	5
Half life in air (h)	2.74E+02	🟩	10
Half life in water (h)	9.96E+01	🟩	10
Half life in soil (h)	1.26E+02	🟩	10

Chemical Status: 🟨

☑ Include Monte Carlo Analysis for Single Chemical

▨ Results already present
🟩 No warnings: calculation possible
🟨 Warnings: calculation still possible
🟥 Errors: calculation impossible
☐ No data entered

Figure 3-2. Screen Capture of OECD Pov and LRTP Screening Tool Parameters Used to Calculate the LRTP of D4

3.1.4 Evidence Integration

A brief description of evidence integration for fate and transport is available in the 2021 Draft Systematic Review Protocol (U.S. EPA, 2021d). The environmental fate characteristics of D4 given in Appendix C of the final scope (U.S. EPA, 2022b) were identified prior to completing the systematic review. Table 3-1 provides selected environmental fate data that EPA considered while assessing the fate of D4 and were updated after publication of the final scope (U.S. EPA, 2022b) with additional information identified through the systematic review process. The following sections summarize the findings and provide the rationale for selecting these environmental fate characteristics.

Table 3-1. Environmental Fate Properties of D4

Property or Endpoint	Value[a]	Reference(s)	Data Quality Rating
Direct photodegradation	Not expected to be susceptible to direct photolysis by sunlight because the chemical structure of D4 does not contain chromophores that absorb at wavelengths >290 nm	Abe et al. (1981)	High
Indirect photodegradation	$t_{1/2}$ = 11.4 days (based on •OH rate constant of 0.94E−12 cm^3/mole-sec at 24 °C and a 12-hour day with 1.5E06 •OH/cm^3)	Atkinson (1991)	High
	$t_{1/2}$ = 8.5 days (based on •OH rate constant of 1.26E−12 cm^3/mole-sec at 24 °C and a 12-hour day with 1.5E06 •OH/cm^3)	Sommerlade et al. (1993)	
	$t_{1/2}$ = 5.1 days (based on •OH rate constant of 2.1E−12 cm^3/mole-sec at 40 °C and a 12-hour day with 1.5E06 •OH/cm^3)	Safron et al. (2015)	
	$t_{1/2}$ = 4.7 days (based on •OH rate constant of 2.3E−12 cm^3/mole-sec at 40 °C and a 12-hour day with 1.5E06 •OH/cm^3)	Xiao et al. (2015)	
	$t_{1/2}$ = 11.3 days (based on •OH rate constant of 0.95E−12 cm^3/mole-sec at 21 °C and a 12-hour day with 1.5E06 •OH/cm^3)	Kim and Xu (2017)	
	$t_{1/2}$ = 10.1 days (based on •OH rate constant of 1.06E−12 cm^3/mole-sec at 21 °C and a 12-hour day with 1.5E06 •OH/cm^3)	Bernard et al. (2018)	
	$t_{1/2}$ = 8.3 days (based on •OH rate constant of 1.3E−12 cm^3/mole-sec at 24 °C and a 12-hour day with 1.5E06 •OH/cm^3)	Alton and Browne (2020)	
Hydrolysis half-life (water)	$t_{1/2}$ = 1.4, 3.4, and 0.02 days at pH 5, 7, and 9, respectively, and 25 °C (OECD 111)	Dow Corning (2004)	High
	$t_{1/2}$ = 22.6 days at 9.5 °C and pH 7 $t_{1/2}$ = 4.2 days at 24.7 °C and pH 7 $t_{1/2}$ = 0.25 days at 9.5 °C and pH 9 (OECD 111)	Durham (2005)	
	$t_{1/2}$ = 15.2, 4.1, 1.6, and 0.4 days at 4, 20, 35, and 55 °C, respectively, and pH 7 (OECD 111)	Gatidou et al. (2016)	
	$t_{1/2}$ = 15.6, 6.3, and 2.3 hours at pH 7.8, 8.5, and 9.2, respectively, and 22 °C	Xu et al. (2016)	
Hydrolysis half-life (soil)	$t_{1/2}$ = 3.5–5.25 days in temperate soil at relative humidity of 32–92%	Xu and Chandra (1999)	High
	$t_{1/2}$ = 4.1–5.3 days in temperate soil at relative humidity of 50–90%	Xu (2007)	

Property or Endpoint	Value[a]	Reference(s)	Data Quality Rating
Abiotic degradation in sediment	$t_{1/2}$ = 49 days in aerobic sediment at 22−25 °C (OECD 308)	Xu and Miller (2008)	High
	$t_{1/2}$ = 365 days in anaerobic sediment at 24 °C (OECD 308)	Xu (2009)	
Aerobic biodegradation in water	3.7%/29 days (OECD 310) at 30.9 mg/L test substance concentration in domestic sludge and soil, adaptation not specified	Gledhill (2005)	High
	0.4%/7 days at 10 mg/L test substance concentration in industrial sludge and soil	Bayer AG (1995)	
Anaerobic biodegradation in sediment	2.1%/29 weeks (OECD 308)	Xu (2009)	High
Bioconcentration factor (BCF) (L/kg wet weight, unless noted)	BCF_{ss} = 5,695 and 11,164 (whole body) at mean test concentration of 29.4 µg/L for 1-g and 5-g rainbow trout (*Oncorhynchus mykiss*), respectively	Dow Corning (1992)	High
	BCF_{ss} = 8,474 (whole body) at mean test concentration of 29.9 µg/L for fathead minnow (*Pimephales promelas*)	Dow Corning (1993a)	
	Mean BCF_{ss} = 12,400 and BCF_k = 13,400 (whole body) at test concentration of 0.5 µg/L for fathead minnow (*Pimephales promelas*)	Fackler et al. (1995); Springborn Laboratories (1991a); Springborn Laboratories (1991b)	
	BCF = 2,864.6 (whole body) for rainbow trout (*Oncorhynchus mykiss*) from ADME-B analysis of feeding study data	Compton (2019)	
	BCF_k = 1,673 (muscle) at mean test concentration of 4.79 ng/L for common carp (*Cyprinus carpio*)	Kim et al. (2020)	
	BCF_{ss} = 1,740 and BCF_k = 2,104 (muscle) at mean test concentration of 4.79 ng/L for common carp (*Cyprinus carpio*)	Xue et al. (2020)	
	BCF = 8,258 and 4,153 (whole body) assuming 2.0 and 7.1 mg-DOC/L, respectively, for rainbow trout (*Oncorhynchus mykiss*) from ADME-B analysis of feeding study data	Cantu et al. (2024)	
Bioaccumulation factor (BAF) (L/kg wet weight, unless noted)	Mean BAF_{ss} = 5,900 (muscle) for crucian carp (*Carassius carassius*)	Guo et al. (2021)	High
	Mean BAF_{ss} = 4,141 (muscle) for crucian carp (*Carassius carassius*)	Wang et al. (2021)	
Organic carbon:water	4.19 ± 0.04 at 24.8 °C (OECD 106)	Miller and Kozerski (2007)	High

Property or Endpoint	Value[a]	Reference(s)	Data Quality Rating
partition coefficient (log K_{OC}) (soil)	4.22 ± 0.05 at 24.4–24.8 °C	Kozerski et al. (2014)	
Organic carbon:water partition coefficient (log K_{OC}) (sediment)	5.17 ± 0.23 at 25 °C	Panagopoulos et al. (2017)	Medium
Dissolved organic carbon:water partition coefficient (log K_{DOC})	5.05 ± 0.07	Panagopoulos et al. (2015)	High
Removal in wastewater treatment	~88% mean total removal from four wastewater treatment facilities	Hydroqual (1993)	High
	98% mean total removal at 11 wastewater treatment facilities	Wang et al. (2013)	
	96% total removal (29% by sludge) at a wastewater treatment facility	Wang et al. (2015a)	
Biota-sediment accumulation factor (BSAF) (g-OC/g-lipid, unless noted)	Mean BSAF = 2.15 ± 1.57, 1.25 ± 0.21, and 0.81 ± 0.27 in sediment with low (0.23%), medium (2.3%), and high (3.9–4.1%) organic carbon content, respectively, for midge (*Chironomus tentans*)	Springborn Laboratories (1991d); Springborn Laboratories (1991e)	High
	Mean BSAF = 2.15 ± 0.64, 1.3 ± 0.00, and 0.7 ± 0.08 in sediment with low (0.23%), medium (2.3%), and high (4.1%) organic carbon content, respectively, for midge (*Chironomus tentans*)	Kent et al. (1994)	
	Mean BSAF = 1.2 in shrimp from inner Oslofjord and 2.6 in shrimp from outer Oslofjord	Evonik Goldschmidt (2009)	
	Mean BSAF = 0.42 ± 0.06 for mollusks (*Mytilus galloprovinvialis*, *Cyclina sinensis*, and *Crassostrea talienwhanensis*)	Zhi et al. (2019)	
Biomagnification factor (BMF) (kg/kg lipid-normalized, unless noted)	1.9–2.4	Dow Corning (2009); Powell et al. (2010)	High
	1–1.4	Dow Corning (2010)	
	0.66 ± 0.21 (OECD 305)	Woodburn et al. (2013)	
	0.35 ± 0.08	Compton (2019)	
	3.2	Xue et al. (2019)	

Property or Endpoint	Value[a]	Reference(s)	Data Quality Rating
	0.444 (± 0.079 SE)	Cantu et al. (2024)	
Trophic magnification factor (TMF)	0.5 and 0.8	Powell et al. (2009)	High
	Pelagic food web: 0.57–0.76	Borgå et al. (2013)	
	0.74	McGoldrick et al. (2014)	
	1.5	Jia et al. (2015)	
	0.6 and 1.3	Powell et al. (2017)	
	Pelagic food web: 0.4–0.7; Demersal food web: 0.5–0.7	Powell et al. (2018)	
	1.7	Cui et al. (2019)	
	0.75	He et al. (2021)	
	0.9	Kim et al. (2022)	

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

3.2 Partitioning

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 are controlled by physical and chemical interactions between D4 and the surrounding media (*e.g.*, air, water, soil, sediments, etc.). D4 released to the environment is subject to these processes with some processes of greater importance than others based on its physical and chemical characteristics (Section 2.2).

To be able to understand and predict the behaviors and effects of D4 in the environment, the first step is identifying the major and minor media compartments and partitioning values (Table 3-2), which can provide insight into how D4 may favor one compartment over another.

Table 3-2. Partitioning Values for D4

Partition Coefficient	Value	Log Value	Source(s)	Predominant Phase
Octanol/water (K_{OW})	9.55E06 at 21.7 °C	6.98 at 21.7 °C	Xu and Kropscott (2012)	Organic carbon
Organic carbon/water (K_{OC})	16,032 at 24.8 °C	4.205 at 24.8 °C	Average of Miller and Kozerski (2007) and Kozerski et al. (2014)	Organic carbon
Octanol/air (K_{OA})	19,498 at 21.7 °C	4.29 at 21.7 °C	Xu and Kropscott (2012)	Organic carbon

Air/water (K_{AW})	490 at 21.7 °C	2.69 at 21.7 °C	Xu and Kropscott (2012)	Air
Soil/water (K_{SW})	2,399	3.38	Bletsou et al. (2013)	Organic carbon

Based on the partition coefficients reported in Table 3-2, D4 will preferentially partition to organic carbon over air and water, and soil over water. This suggests that the major environmental compartments for D4 will be air, soil, biosolids, and sediment.

D4 exists in both gaseous and particulate phases in the atmosphere (Anh et al., 2021; Tran and Kannan, 2015; Tran et al., 2017; Li et al., 2020). A log K_{OA} value of 4.29 indicates that D4 will favor organic carbon over air (Table 3-2). However, higher D4 concentrations were measured in gaseous phase compared to particulate phase (Tran and Kannan, 2015). The AEROWIN™ program in EPI Suite™ estimated that a negligible fraction (8×10^{-5} to 2×10^{-3} percent) of D4 may be sorbed to atmospheric particulates (U.S. EPA, 2017). Thus, D4 is expected to have a low tendency to associate with particulates and will predominately be in the gaseous phase (ECHA, 2012; Xu and Wania, 2013; Surita and Tansel, 2014; NICNAS, 2020). The gaseous-particulate distribution of D4 may change depending on the relative humidity as well as temperature (Anh et al., 2021). Given the volatility of D4 and the expectation that releases will be primarily to air and water, air is expected to be a major compartment for D4.

Down-the-drain disposals from industrial and consumer uses are a primary source of D4 in water compartments. While much of D4 is expected to either volatilize or sorb to sludge during wastewater treatment, quantifiable levels may be present in the effluent (Wang et al., 2013; Zhang, 2014). A log K_{AW} value of 2.69 indicates that D4 will favor air over water (Table 3-2), which means D4 is expected to readily evaporate from water and moist soil into the atmosphere. D4 does not appreciably partition to water due to its water solubility (0.056 mg/L at 23 °C) (Dow Corning, 1991; Varaprath et al., 1996; NCBI, 2021), so volatilization is expected to be a dominant pathway for D4 (Chandra, 1997; ECHA, 2012; Shoeib et al., 2016). In addition, D4 may hydrolyze to smaller, more polar products in water. Thus, surface water is a minor compartment for D4.

3.2.2 Tier II Analysis

This Tier II analysis was conducted to identify the fate pathways and media most likely to cause exposure to environmental releases and which media should be emphasized during evaluation. For the air compartment, the greatest half-life from Atkinson (1991) was selected as the best value for a conservative approach. Since hydrolysis was the dominant pathway for D4 degradation in surface water, the selected water half-life is an average of the hydrolysis half-lives obtained from two OECD TG 111 studies (Durham, 2005; Gatidou et al., 2016). For the soil compartment, the empirical half-life from Xu and Chandra (1999) was selected. The sediment half-life is an average of the half-lives obtained from three OECD TG 308 studies (Xu and Miller, 2008; Xu, 2009; Xu and Miller, 2009). All the half-life values were obtained at environmental conditions (*i.e.*, pH 7 and 22–25 °C). All other input variables were left at their default settings (*e.g.*, equal emission rates and advection time). Table 3-3 lists the half-life inputs used for the LEV3EPI™ runs.

Table 3-3. Environmental Half-Lives Used in EPI Suite™ Level III Fugacity Modeling

Media	Half-Life (hours)	Reference(s)
Air	273.6	Atkinson (1991)

Media	Half-Life (hours)	Reference(s)
Water	99.6	Average of Durham (2005) and Gatidou et al. (2016)
Soil	126	Xu and Chandra (1999)
Sediment	5,248	Average of Xu and Miller (2008), Xu and Miller (2009), and Xu (2009)

Assuming equal releases to air, water, and soil, the LEV3PI™ results show that D4 emissions will primarily partition to air (52%), water (30%), and sediment (16%) with 2 percent to soil (Table 3-4; Figure 3-3). These results reiterate the Tier I analysis results that air is expected to be a major compartment for D4 released to the environment. Though the expected lifespan of D4 in water is short based on its physical and chemical properties that drive rapid volatilization and hydrolysis, the sizable 30 percent fraction predicted to be in aqueous media may be inflated by predictions of sorption to particulate matter in the water column.

Table 3-4. EPI Suite™ Level III Fugacity Modeling Results for D4

Substance Released to	Percentage (%) of Substance Partitioning into Each Compartment			
	Air	Water	Soil	Sediment
100% Soil release	90.5	0	9.5	0
100% Air release	100	0	0	0
100% Water release	9.9	58.6	0	31.5
Equal releases	52	30	2	16

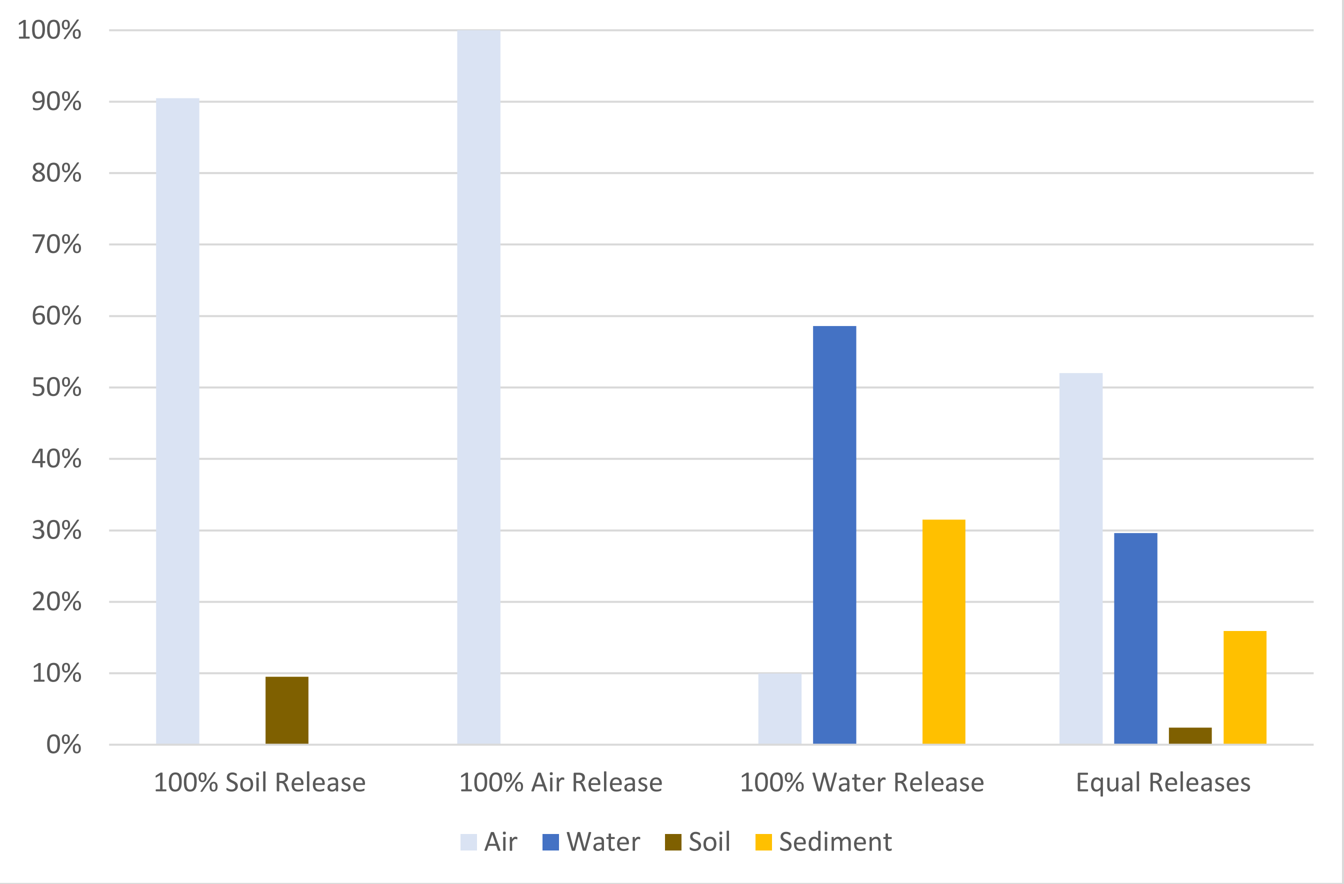


Figure 3-3. EPI Suite™ Level III Fugacity Modeling Graphical Result for D4

3.3 Transformation Processes

3.3.1 Hydrolysis

Hydrolysis is 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 both how long the chemical and/or its hydrolysis byproducts will remain after being released to the environment.

3.3.1.1 Surface Water

Hydrolysis is the dominant pathway for D4 degradation in surface water. D4 is expected to undergo rapid hydrolysis, and its hydrolysis rate is dependent on the pH and temperature. D4 hydrolysis proceeds from a ring-opening step, forming tetramer diol that will subsequently hydrolyze to form trimer and dimer diols, terminating with DMSD (Dow Corning, 2004; Durham, 2005; Gatidou et al., 2016). Five high-quality hydrolysis studies were identified during systematic review.

Three studies determined the hydrolysis rates of D4 using OECD TG 111 that was modified to consider the volatility of D4. Dow Corning (2004) conducted sealed tube hydrolysis studies at 25 °C and pH levels 5, 7, and 9. Base catalysis was the more efficient mechanism ($t_{1/2}$ = 0.56 hours at pH 9), followed by acid catalysis ($t_{1/2}$ = 33 hours at pH 5). Hydrolysis of D4 under neutral conditions was much slower ($t_{1/2}$ = 69 hours at pH 7), demonstrating the parabolic nature of D4's hydrolysis with respect to pH. Durham (2005) conducted experiments at pH 4, 7, and 9, and temperatures at 10, 25 and 35 °C. In agreement with Dow Corning (2004), the slowest hydrolysis rate was observed at pH 7 ($t_{1/2}$ = 101.6

hours at 25 °C), followed by pH 4 ($t_{1/2}$ = 1.77 hours at 25 °C), and pH 9 ($t_{1/2}$ = 0.96 hours at 25 °C). Across all pH tests, hydrolysis rates increased with temperature. The shortest observed half-life was 0.19 hours at pH 9 and 35 °C, while the longest was 542 hours (≈ 22.6 days) at pH 7 and 10 °C. Gatidou et al. (2016) assessed D4 hydrolysis in amber glass vials at 4, 20, 35, and 55 °C. As anticipated, the slowest hydrolysis occurred at 4 °C with a half-life of 15.2 days (≈ 365 hours), and the fastest at 55 °C with a half-life of 0.4 days (≈ 9.6 hours). However, there is additional uncertainty in these half-lives since the test concentration was 100 µg/L, which is almost double D4's water solubility with no additional detail on D4 recovery from the buffer matrix or how D4 degradation was determined. In addition, all three studies reported DMSD and its oligomers as the byproducts of D4 after undergoing hydrolysis (Dow Corning, 2004; Durham, 2005; Gatidou et al., 2016).

A non-guideline study, Xu et al. (2016) used a lower D4 concentration of 0.5 µg/L at 22 °C over 48 hours at various pH levels. The mean half-lives were 15.6, 6.32, and 2.33 hours at pH 7.8, 8.5, and 9.2, respectively. This generally supports the OECD TG 111 studies and demonstrates hydrolysis at a more environmentally relevant concentration in alkaline systems. Xu et al. (2016) also identified DMSD as a hydrolysis byproduct of D4.

Dow Chemical (2022a) used the data from Durham (2005) to model the pseudo first-order rates of hydrolytic and condensation reactions governing concentrations of DMSD oligomer hydrolysis products. Rate constant k_4 was found to be much slower than k_3, indicating that the top pathway is dominant (Figure 3-4). Half-lives of 6.9, 8.2, and 7.3 days were calculated for the tetramer, trimer, and dimer diol oligomers, respectively, at pH 7 and 25 °C showing low aqueous persistence.

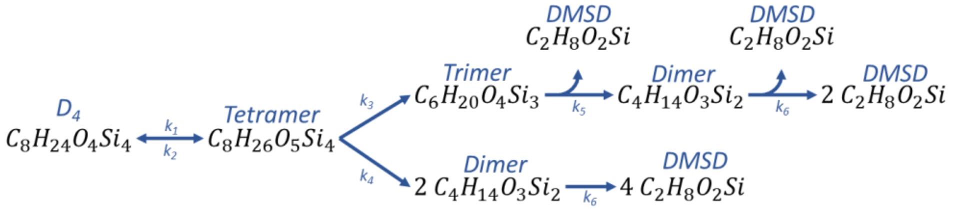


Figure 3-4. Summary of D4 Hydrolysis Pathway Showing Stoichiometric Ratios Among the Silanols Adapted from Dow Chemical (2022a)

A medium-quality study, Spivack and Dorn (1994) determined the hydrolytic equilibrium between DMSD, dimer, and trimer diols. The stability of DMSD in aqueous media was seen to be much greater than for D4 and the other oligomers, as discussed in Appendix A.2.1.1.

3.3.1.2 Sediment

Three high-quality microcosm studies demonstrated abiotic hydrolysis of D4 in sediment (Xu and Miller, 2008; Xu, 2009; Xu and Miller, 2009). In Xu and Miller (2008), approximately 32 percent of D4 underwent hydrolysis after 22 days under aerobic conditions. D4's half-life was calculated to be approximately 47 days and the degradation products identified as silanediol and siloxanediols. However, the complete mineralization of either D4 or its hydrolytic products to CO_2 was not significant (<0.15%) after the first three weeks. Another aerobic study, Xu and Miller (2009), reported a D4 sediment half-life of 242 days. Concurrent tetramer, trimer, and dimer silanol formation and subsequent hydrolysis were observed early in the experiment (<7 days), leaving the dominant DMSD product through the end of the study. Xu (2009) reported a calculated half-life of 365 days under anaerobic conditions and D4 was seen to hydrolyze to the same silanols terminating with DMSD.

3.3.1.3 Soil

Four high-quality studies investigating the removal mechanisms of D4 in soil were identified during systematic review. Xu and Chandra (1999) examined hydrolysis in two different soils. One was a temperate soil, Londo, with a pH of 7.6, organic matter content of 2.4 percent, and consisted of 50 percent sand, 28 percent silt, and 22 percent clay. The other soil was a highly weathered Hawaiian soil, Wahiawa, with a pH of 4.9 and organic matter content of 2.2 percent, and consisted of 21.2 percent sand, 24 percent silt, and 54.8 percent clay. The experiments were conducted in both open and closed tubes at 22.2 °C under different relative humidities (32, 92, and 100 percent) for seven days. The half-lives for D4 in Londo soil were 3.54 and 5.25 days at relative humidity of 32 and 92 percent, respectively. Little or no degradation of D4 was observed at 100 percent relative humidity. The half-lives for D4 in Wahiawa soil were 0.04 days (≈ 58 minutes), 0.08 days (≈ 1.9 hours), and 0.89 days (≈ 21 hours) at relative humidity of 32, 92, and 100 percent, respectively. Xu and Chandra (1999) described the degradation as a multi-step hydrolysis that was initiated with the ring-opening hydrolysis, like in water and sediment. The ultimate degradation product was DMSD. These findings suggest that the rate of degradation decreases as the soil moisture increases and the degradation rate was faster in weathered soil due to its higher pH and clay content. Volatilization was seen to be negligible at low moisture levels due to high sorption and fast degradation of D4 in dry soil. But when degradation rates were low at higher relativity humidity, volatilization accelerated and was the predominant process.

Xu (2007) performed a data extrapolation based on the measured hydrolysis rates of D4 in two soils from Xu and Chandra (1999) and Xu (1999) to estimate the soil degradation rate at three different moisture levels (50, 70, and 90%). The extrapolated half-lives for Londo soil were 4.1, 4.7, and 5.27 days at relative humidity of 50, 70, and 90 percent, respectively. The extrapolated half-lives for Wahiawa soil were 0.046 days (≈ 1.1 hours), 0.06 days (≈ 1.44 hours), and 0.078 days (≈ 1.87 hours) at relative humidity of 50, 70, and 90 percent, respectively. These results agree with the results reported by Xu and Chandra (1999).

Two high-quality field studies, Shi et al. (2015) and Xu, L. et al. (2019) conducted a simulated hydrolysis study using uncontaminated soil that was mixed with crude oil and petroleum ether to determine whether petroleum hydrocarbons had an effect on the hydrolysis kinetics of D4. Both studies were excluded from use in this risk evaluation because soil with crude oil does not represent D4’s behavior in natural soil.

The formation of silanols and DMSD in soil is not exclusive to D4 degradation. DMSD and linear silanols were shown to be formed from D5 and dodecamethylcyclohexasiloxane (D6) hydrolysis in soil (Xu, 1999; Xu and Chandra, 1999), along with the hydrolysis of PDMS in various soil and sludge systems (Lehmann et al., 1994a, 1994b; Carpenter et al., 1995; Lehmann et al., 1995; Lehmann and Miller, 1996; Lehmann et al., 2000, 2002). The fate of DMSD is discussed further in Appendix A.2.1.1.

3.3.2 Biodegradation

Biodegradation occurs when an organic material is broken down by biological microorganisms under natural environmental conditions (*i.e.*, aerobic and anaerobic).

3.3.2.1 Surface Water

D4 is not expected to biodegrade rapidly in surface waters under environmentally relevant conditions. Gledhill (2005) performed an OECD TG 310 sealed vessel headspace carbon dioxide (CO_2) evolution biodegradation test for D4 ready biodegradability. An inoculum was prepared from a municipal wastewater treatment plant (WWTP) sludge and sewage, and fresh soil was added at 10 mg/L. The test showed 3.7 percent degradation of D4 at day 29 (the maximum degradation was 16.2 percent at day

21).[2] However, there is uncertainty regarding this study. The D4 concentration was several orders of magnitude above its water solubility, which likely does not represent the bioavailability of D4.

This result is supported by a set of non-test guideline studies performed by Bayer AG (1995) using inocula from two German WWTPs treating chemical industry waste in Leverkusen and Dormagen. No CO_2 evolution was observed after one week of incubation.

3.3.2.2 Sediment

In sediment, the half-life of D4 is long, qualifying it as highly persistent (64 FR 60194, November 4, 1999). Three high-quality studies used OECD TG 308 (OECD, 2002) to measure anaerobic and aerobic transformation of D4 in freshwater sediment systems, with modifications to minimize the effects of D4 volatility on the accuracy of the tests.

Springborn Laboratories (1991c)[3] used core chambers, which are laboratory microcosms that simulate natural conditions, to study the biodegradation of test materials in certain lentic environments. Water and sediment samples were collected from Horseshoe Pond located in Wareham, Massachusetts. The sediment had a pH of 5.5 and 3.2 percent organic carbon (OC) content, and consisted of 74 percent sand, 22 percent silt, and 4 percent clay. No indication of biodegradation was observed after a 28-day study with a ^{14}C-D4 dose of 32.2 µg/L to the water fraction. The largest ^{14}C percentage was recovered from volatile organic carbon (VOC) traps, followed by sediments, then water. Parent D4 accounted for less than one percent of ^{14}C both water and sediment at the conclusion of the study, indicating extensive hydrolysis in both compartments. However, two specifics from this study introduce high uncertainty, as discussed in Brooke et al. (2009c). Firstly, the mass balance varied greatly, ranging between 47.3 and 101.6 percent and the mean recovery values were below 80 percent. Secondly, the ^{14}C-D4 concentrations measured in the sediment varied greatly in replicates for the same sampling time.

Xu (2009) studied the degradation rates of D4 under anaerobic conditions with sediment from Lake Pepin, which is located on the border between Minnesota and Wisconsin. At a pH of 7.9 and an average test temperature of 24 °C, D4 loss was negligible (97.9 percent remaining after 29 weeks), which corresponds to a half-life of 365 days. Xu and Miller (2009), an accompanying aerobic study with Lake Pepin sediment, yielded a half-life of 242 days. Hydrolysis products were detected in the aerobic study, though complete mineralization/CO_2 generation was less than one percent over 22 weeks. Xu and Miller (2008) conducted an aerobic degradation study with sediment from Sanford Lake in Michigan and obtained a much shorter half-life of 47 days. Again, the primary transformation mechanism was hydrolysis with a 32 percent loss of D4 within 22 days, though with less than 0.15 percent mineralization. The stark contrast between the aerobic half-lives from Xu and Miller (2008, 2009) can be explained by several factors. Firstly, the Sanford Lake sediment test was conducted at a pH of 6.95, which was approximately one unit lower than Lake Pepin. Secondly, the Sanford Lake sediment contained about one percent lower OC content. Thirdly, as discussed in Section 3.3.1.1, D4 hydrolyzes more rapidly under basic conditions (Dow Corning, 2004; Durham, 2005). Lastly, a higher sediment OC content can reduce hydrolysis transformation by D4 sorption to sediment organics.

3.3.2.3 Soil

One high-quality biodegradation study on D4 was identified during systematic review. Dow Corning (1997) reported that more than 99 percent of D4 was degraded in highly weathered soil at 100 percent

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[2] The apparent decrease in CO_2 evolution in the treatment vials is likely due to a gradual increase in CO_2 in the abiotic controls between day 21 and 29, and due to natural variance among all vessels.

[3] Technology Sciences Group (1997) is the same study as Springborn Laboratories (1991c). Therefore, it is not discussed in this assessment.

relative humidity within 24 hours and a large of fraction of degradation product was DMSD. It is highly likely that D4 did not undergo biodegradation but instead was hydrolyzed (see Section 3.3.1.3).

3.3.3 Photolysis

Photolysis is another form of chemical reaction in which chemical molecules are broken down after absorbing light, primarily in the ultraviolet range. There are two forms of photolysis: direct and indirect. Direct photolysis occurs when a chemical substance interacts directly with the sunlight, while indirect photolysis occurs in the presence of photosensitizers (*e.g.*, ozone (O_3), nitrate (N_3), and hydroxyl radicals (•OH), etc.) under visible light.

3.3.3.1 Atmosphere

Direct Photodegradation

D4 is not expected to undergo significant direct photolysis in the atmosphere since its chemical structure does not absorb light at wavelengths greater than 290 nm (Abe et al., 1981).

Indirect Photodegradation

D4 in the gaseous phase is expected to degrade slowly by reaction with photochemically produced hydroxyl radicals (•OH) in the atmosphere. Assuming 12 hours of light reaction, a hydroxyl (OH) concentration of 1.5×10^{6} OH/cm^3, and rate constants ranging from 0.94×10^{-12} to 2.3×10^{-12} cm^3/molecule-second, the measured atmospheric half-lives for D4 ranged from 4.7 to 11.4 days (Atkinson, 1991; Sommerlade et al., 1993; Safron et al., 2015; Xiao et al., 2015; Kim and Xu, 2017; Bernard et al., 2018; Alton and Browne, 2020). Degradation by reactions with nitrate radicals (•NO_3) and ozone radicals (•O_3) were seen to be negligible (Abe et al., 1981; Atkinson, 1991; U.S. EPA, 2017). Since its estimated atmospheric half-lives are greater than two days, D4 meets the criterion for persistence in the air compartment (64 FR 60194, November 4, 1999). The atmospheric half-life of D4 does not pertain to indoor environments due to lower •OH concentrations, less mixing of air, and lower sunlight intensity.

Sommerlade et al. (1993) identified heptamethylhydroxycyclotetrasiloxane ($C_7H_{22}O_5Si_4$; CASRN 5290-02-8) (19.95% of the total amount of GC-detectable substances) as the major degradant from the reaction of D4 with •OH, along with lesser amounts of heptamethyl(hydroperoxymethyl)cyclotetrasiloxane ($C_8H_{24}O_6Si_4$; CASRN 150375-95-4) (9.95%), 1,2-bis(heptamethylcyclotetrasiloxanyl)ethane ($C_{16}H_{46}O_8Si_8$; CASRN 17156-73-9)(4.22%), heptamethyl(hydroxymethyl)cyclotetrasiloxane ($C_8H_{24}O_5Si_4$; CASRN 17866-06-7) (0.74%), and bis(heptamethylcyclotetrasiloxanyl)ether ($C_{14}H_{42}O_9Si_8$; CASRN 17909-39-6) (0.72%). The hydroxyl-substituted degradation products are likely to be removed from the atmosphere by wet deposition because they are expected to be more soluble in water and have a lower vapor pressure than D4 (Chandra, 1997; Brooke et al., 2009c; Janechek et al., 2017; Alton and Browne, 2022).

Navea et al. (2009) developed a box model to simulate D4 concentration by mass balance, using three different atmospheric segments (urban, suburban, and rural) to simulate their population density, emissions, and OH concentrations in the summertime. This study was not used in this risk evaluation because multiple high-quality empirical data on indirect photodegradation are available.

A half-life of 8.55 days was calculated from the Atmospheric Oxidation Program (AOPWIN™) in EPI Suite™ using an estimated rate constant of 2.25×10^{-12} cm^3/molecule-second at 25 °C, assuming an atmospheric •OH concentration of 1.5×10^{6} molecule/cm^3 and a 12-hour day (U.S. EPA, 2017). The result from AOPWIN™ was not selected for use in this risk evaluation because high-quality empirical data on indirect photodegradation are available.

3.3.3.2 Surface Water

A medium-quality study examining direct photolysis of D4 in water was identified during systematic review. Dow Corning (1980) reported that D4 underwent photolytic oxidation on water containing 10 ppm nitrate ion in the presence of simulated sunlight. Visible films of D4 shrank and gel was formed on the surface of water when exposed to light. Because Dow Corning (1980) investigated a D4 film (neat) rather than aqueous phase D4, the findings are not relevant to D4 in the environment. Therefore, this study was excluded for use in this risk evaluation. No other information is available on the direct photolysis of D4 in water. D4 is not expected to undergo aqueous photolysis since hydrolysis is expected to be the main degradation pathway in water. Indirect aqueous photolysis is not expected to contribute to D4 transformation in water due to its general low susceptibility to indirect photolytic processes in the atmosphere (see Section 3.3.3.1).

3.4 Media Assessments

D4 has been detected in the atmosphere, and aquatic and terrestrial environments. In the air, D4 will be most predominant in the gaseous phase and is expected to be persistent (64 FR 60194, November 4, 1999). D4 was detected in indoor air and dust and is strongly correlated with occupant density. D4 is expected to have a longer half-life in indoor air compared to outdoor air due to lower •OH concentrations, less mixing of air, and lower sunlight intensity. In aquatic environments, D4 does not undergo biodegradation in water and is expected to hydrolyze rapidly. D4 can be transported to sediments from overlying surface water via advection, dispersion, and sorption to suspended solids that can settle out from the water column. D4 will have a strong affinity for organic carbon in sediment. In terrestrial environments, D4 may be present in soils via land-application of biosolids. However, D4 is unlikely to migrate to groundwater and surface water via runoff because D4 is expected to dissipate in the soil via abiotic processes such as hydrolysis and volatilization.

3.4.1 Air and Atmosphere

3.4.1.1 Outdoor Air

D4 is expected to have a low tendency to associate with particulates and will predominately be in the gaseous phase (see Section 3.2.1). Generally, higher concentration of D4 is expected to be found in the gaseous phase than in particulate phase. Tran and Kannan (2015) reported a maximum D4 air concentration of 722 ng/m^3 in the gaseous phase, while the maximum D4 air concentration in particulate phase was 101 ng/m^3.

Due to its widespread use and high volatility, a large fraction of D4 is released into the air during manufacture, use and recycling/disposal processes (Kaj et al., 2005a; Ahrens et al., 2014; Companioni-Damas et al., 2014; NICNAS, 2020). There is a greater tendency for D4 air concentrations to be higher in urban and industrial areas compared to suburban and rural areas. D4 air concentrations were detected up to 0.19 µg/m^3 in Chicago, while the maximum concentrations of 0.014 and 0.037 µg/m^3 in were measured in a rural and suburban areas in Iowa, respectively (Yucuis et al., 2013). Several other air monitoring studies also observed the general trend of increasing air concentrations with increasing population density (Wang et al., 2001; Genualdi et al., 2011; Jiang, 2022). Additional sources of D4 air emissions are landfills and WWTPs (see Sections 3.4.3.3 and 3.5.2). The highest D4 air concentration was measured near an aeration tank (up to 2.11 µg/m^3) in a WWTP and a landfill (up to 0.471 µg/m^3) in Ontario, Canada (Cheng et al., 2011).

Based on its physical and chemical properties and long half-life in the atmosphere ($t_{1/2}$ = 4.7–11.4 days), D4 is assumed to be persistent in the air (see Section 3.3.3.1). The OECD P_{OV} and LRTP Screening Tool was run to get additional information on D4's long-range transport potential in the air. For D4 emissions in air, a P_{OV} of 16 days, CTD of 5,658 km (≈ 3,515.7 miles), and TE of 0.0184 percent were given using a molecular mass of 296.61 g/mol, log K_{AW} of 2.69, and log K_{OW} of 6.488 along with an atmospheric half-life of 273.6 hours, a water half-life of 99.6 hours, and soil half-life of 126 hours (Table 3-3; Figure 3-2). A CTD of 5,658 km suggests that D4 does have the potential to undergo long-range transport in the air (*e.g.*, 1,936 km from Washington, D.C. to Arctic Ocean), however a TE of 0.0184 percent suggests that a negligible fraction of D4 emitted to air will be deposited to surface media such as water. CTD can also be calculated using the LEV3EPI™ model in EPI Suite™ without considerations for advection (Beyer et al., 2000; U.S. EPA, 2017). After entering the physical and chemical properties of D4 (Figure 3-1), a CTD of 4,680 km (≈ 2,908 miles) was calculated. Both modeling results confirm that D4 has the potential to undergo atmospheric long-range transport.

3.4.1.2 Indoor Air and Dust

D4 can be released to indoor air, either as an impurity from silicone-containing products (*i.e.*, electrical and electronic devices, building materials, paints and coatings, sealants, etc.) or during the use of cosmetics and personal care products (Lu et al., 2010; Gallego et al., 2017; Shen et al., 2018; Tran et al., 2019; Zhu et al., 2023).

Concentrations of D4 in indoor air was observed to be higher than those in outdoor air. For instance, Yucuis et al. (2013) reported a maximum outdoor air concentration of 0.37 $\mu g/m^3$ compared to a maximum indoor air concentration of 0.5 $\mu g/m^3$ in an office. D4 was also detected in indoor dust samples (Lu et al., 2010; Xu et al., 2012; Meng and Wu, 2015; Tran et al., 2015; Zhu et al., 2023), at levels as high as 17 $\mu g/m^3$ in a barbershop (Liu et al., 2017). Studies have demonstrated that D4 concentrations in indoor air were observed to have strong correlation with occupant density (Shields et al., 1996; Yucuis et al., 2013). In addition, out of all microenvironments studied, D4 concentrations in dust generally decreased in the order: barbershops/beauty salons > homes > offices > laboratories as a result of certain products being used (Sha et al., 2018; Anh et al., 2021; Lu et al., 2010; Yucuis et al., 2013; Companioni-Damas et al., 2014; Tran and Kannan, 2015; Liu et al., 2017).

3.4.1.3 Key Sources of Uncertainty in the Assessment of Air and Atmosphere

Since the assessment of the fate of D4 in air and atmosphere relied on empirical •OH oxidation half-lives from multiple high-quality studies (see Section 3.3.3.1), there is a robust confidence that D4 is persistent (64 FR 60194, November 4, 1999) and may undergo atmospheric long-range transport. In addition, there are several non-TSCA uses of D4 (*i.e.*, cosmetics and personal care products) that are released to the air. It is not possible to differentiate whether the releases were directly from TSCA or non-TSCA uses.

3.4.2 Aquatic Environments

D4's presence in aquatic environments is primarily due to releases from industrial processes, down-the-drain disposals from industrial and consumer uses, and non-point sources especially from urban areas (EC/HC, 2008c; Horii and Kannan, 2008; Genualdi et al., 2011; Lee et al., 2019; NICNAS, 2020).

3.4.2.1 Surface Water

Environmental concentrations of D4 are generally higher near industrial processing facilities (Zhang et al., 2018; Jiang, 2022), in waters receiving WWTP effluent (Schlabach et al., 2007; Dow Corning, 2010; Horii et al., 2017; Jiang, 2022), and near densely populated and coastal areas (Anh et al., 2021; Hong et al., 2014; Powell et al., 2017). The main removal mechanisms of D4 are volatilization from water during aeration and adsorption onto sludge (see Section 3.5.2), however a fraction of D4 will be discharged into receiving waters.

Concentrations of D4 in surface water in the United States and Canada were reported in three studies (Simon and Paulson, 1985; Wang et al., 2013; ERM, 2017a). Simon and Paulson (1985) collected samples of final effluent from three WWTPs and reported D4 concentrations at below detection limits (<0.5 µg/L) for all sites (Ann Arbor, Detroit, and Washington, D.C.). Wang et al. (2013) reported D4 concentrations up to 0.023 µg/L in waters receiving effluents of nearby WWTPs in Canada. The environmental testing program (ERM, 2017a, 2017b) collected environmental media samples from fourteen WWTPs located in New York, Michigan, Ohio, West Virginia, Kentucky, Illinois, Kansas, Iowa, Colorado, and Oregon during two sampling events between 2016 to 2017. Four WWTPs were manufacturing/processing plants that treated wastewater onsite and discharged directly into a receiving water body under a National Pollution Discharge Elimination System (NPDES) (referred to as direct discharge or "DD" WWTPs). Five WWTPs received wastewater for treatment from industrial sites known to be D4 processors or formulators (referred to as indirect discharge or "I" WWTPs). The other five WWTPs received less than 15 percent of wastewater for treatment from industrial facilities that were not D4 manufacturing, processing, or formulating sites (referred to as non-industrial or "R" WWTPs). Surface water samples were collected from the midpoint of the edge of the adequately mixed zone. The highest concentration was 0.7 µg/L at the location in Friendly, WV where D4 was detected at 100 percent. D4 was not detected in surface water samples from the indirect WWTPs. For the non-industrial WWTPs, D4 was found in most samples at one location (Genesee, MI) during the first sampling event, but levels were below the laboratory method detection limit (<0.037 µg/L) during the second event. D4 was not detected in the remaining "R" WWTPs.

Bioavailability of D4 to biota in the surface water compartment is expected to be variable and location dependent. An environmental exposure study was conducted at an environmentally relevant concentration (4.79 ± 1.19 ng/L) and reported an uptake rate (k_1) of 199/day in common carp (*Cyprinus carpio*) (Xue et al., 2020). This is an order of magnitude lower than another environmental exposure study that had an uptake rate of 2,450 per day for fathead minnow (*Pimephales promelas)* at a nominal exposure concentration of 500 ng/L, which is approximately 5- to 100-fold greater than observed ambient levels (Fackler et al., 1995). Because of this, D4 is expected to accumulate readily to fish in the water column, especially in environments with greater D4 concentrations such as those receiving WWTP effluent and urban areas releasing non-point source of D4 (EC/HC, 2008c; Warner et al., 2014; Zhi et al., 2019). In remote areas where D4 concentrations are lower and detections are diffuse, it is highly possible that D4 will volatilize due to its Henry's law constant (11.8 atm·m^3/mol at 21.7 °C (Xu and Kropscott, 2012, 2014)), hydrolyze, and/or partition to sediments (log K_{OC} = 5.20 at 25 °C (Panagopoulos et al., 2017)) rather than appreciably partition to biota (see Section 3.6).

The OECD P_{OV} and LRTP Screening Tool was run to get additional information on D4's LRTP in water (Figure 3-2). For D4 emissions in water, a P_{OV} of 6.3 days, CTD of 9.9 km (≈ 6.15 miles), and TE of 2.45×10^{-5} percent were calculated. A CTD of 9.9 km suggests that D4 does not have the potential to undergo long-range transport in water (*e.g.,* 1,963 miles from Washington, D.C. to Arctic Ocean). The persistence of D4 in the surface water compartment is expected to be hydrolysis mediated. Aquatic biodegradation of D4 is expected to be much slower than hydrolytic degradation (see Sections 3.3.2.1 and 3.3.1.1). Given the range of empirical hydrolysis half-lives, D4 is not expected to be persistent ($t_{1/2}$ < 60 days) in the surface water compartment under environmentally relevant conditions.

Hamelink et al. (1996) determined the volatilization rate constant of D4 from water. The volatilization rate constant for D4 was estimated to be 0.005 to 0.22 per hour in rivers and 0.002 to 0.005 per hour in lakes and ponds. The calculated volatilization half-lives of D4 from a 1-meter-deep water body are 3 to 138 hours in rivers and 138 to 145 hours in lakes and ponds. This suggests that D4 will readily volatilize from water. Moreover, Yaman et al. (2020) studied the air-water exchange patterns of D4 in a river basin located in the southwestern part of Turkey. D4 concentrations measured in the air and water samples were used to estimate the net air-water exchange fluxes. The fluxes were negative in all samples, which indicate volatilization from water.

The volatilization half-lives of D4 from a model river and lake were estimated using the Water Volatilization program (WVOLWIN™) in EPI Suite™ and default settings were applied (see default settings in Figure 3-1). The volatilization half-life of D4 was 1.76 and 163.6 hours (≈ 6.82 days) for a model river and lake, respectively (U.S. EPA, 2017). This result agrees with the findings of Hamelink et al. (1996) and Yaman et al. (2020) that D4 is highly likely to volatilize rapidly from water.

3.4.2.2 Sediments

D4 can be transported to sediments from overlying surface water via advection, dispersion, and sorption to suspended solids that settle out from the water column. With D4's log K_{OC} value of 5.20 at 25 °C for lake sediment (Panagopoulos et al., 2017), and a log K_{OW} value of 6.488 at 25.1 °C (Kozerski and Shawl, 2007), D4 will have a strong affinity for OC in sediment. In addition, Panagopoulos et al. (2015) reported a measured log K_{DOC} value of 5.05 ± 0.07, which suggests that D4 is more likely to bind to dissolved organic matter and be less mobile in the water column.

Based on sediment monitoring studies, elevated D4 concentrations were observed near outlets of WWTPs (Schlabach et al., 2007; Shoeib et al., 2016; ERM, 2017a) and industrial areas (Zhang et al., 2018; Lee et al., 2019; Nguyen et al., 2022). Jiang et al. (2022) reported a maximum D4 concentration of 55.3 ng/g dry weight (dw) at a sampling site in Zhangjiagang, where China's largest siloxane production plant is located, and 8.50 ng/g dry weight (dw) near WWTP effluent discharge locations in Beijing and Kunming. D4 concentrations were measured up to 1.20 ng/g dw in other sampling sites that were not impacted by the plant or effluent discharge. Dow Corning (2007) reported a maximum D4 concentration of 286 ng/g dw at a sampling site in Toronto Harbor, which is known to receive direct discharges of treated wastewater. Sediment samples collected as part of the ECA were collected either "very near" and "as close as practicable" to the surface water sampling locations (ERM, 2017a). D4 was detected in all sediment samples collected in a water body that received direct discharges from WWTPs that treat wastewater from D4 manufacturing and processing facilities in the United States. The maximum level (18,000 ng/g dw) was measured at Waterford, NY where samples were collected approximately 60 m downstream from the effluent outfall. For the indirect and non-industrial WWTPs, results varied. Of the ten indirect and non-industrial WWTPs, D4 was detected at a maximum concentration of 7.7 ng/g dw.

In addition, sediment concentrations near populated areas were observed to be higher when compared to rural and/or secluded areas (Dow Corning, 2010; Hong et al., 2014; Zhang et al., 2018). Dow Corning (2009) reported a D4 mean concentration 0.37 ng/g wet weight (ww) in a remote Lake Opeongo, Canada. However, all nine samples were measured below the method detection level (MDL).

3.4.2.3 Key Sources of Uncertainty in the Assessment of Aquatic Environments

Accounting for D4's low solubility, high volatility, ubiquitous use, and high tendency to sorb to particulate matter in field studies can be difficult. Due to this, D4 measurements in aquatic environments often come with caveats of low detection and quantitation frequencies (Schlabach et al., 2007; Dow Corning, 2009; Powell et al., 2009; Dow Corning, 2010; Warner et al., 2010; Horii et al., 2013; Hong et al., 2014; Warner et al., 2014; Powell et al., 2017; Zhi et al., 2018; Norwegian Environment Agency, 2019; Panagopoulos Abrahamsson et al., 2020; Jiang, 2022; Kim et al., 2022), substantial contamination levels (Dow Corning, 2009; Nusz et al., 2018; Kim et al., 2022), and low spike recoveries (Dow Corning, 2009; Wang et al., 2010; Jiang, 2022; Kim et al., 2022). Low detection frequencies driven by high background levels introduce uncertainty, especially in the lower bounds of environmental concentrations of D4. In addition, variation in aqueous concentration is also introduced based on extraction protocol–some studies capture D4 in both dissolved and particulate phases filter samples prior to extraction. Lastly, monitoring concentrations of DMSD within the context of this risk evaluation should be regarded with caution, as DMSD is not formed in the environment solely from TSCA-defined conditions of use for D4.

One of the most significant release sources of D4 into the aquatic environments is down-the-drain discharge from consumer products consumed by the general public (Horii and Kannan, 2008; Xu et al., 2013; Zhang et al., 2018). D4 concentrations in aquatic environments may vary with location, depending on the concentration of D4 in products and the consumption level of users.

The relative contributions of the competing processes of D4 fate in surface waters are further dependent on processes such as advection, turbulence (sediment-water and air-water mixing), biota habitat and habitat range. Therefore, it is expected that exposure to D4 in surface water will be variable and context specific, with greater probability of exposure near WWTP effluent discharge locations and near greatly urbanized areas.

There is some uncertainty over the actual concentration of D4 present in the sediment phase. Sediment concentrations have been demonstrated to be correlated with sediment OC content (Zhang et al., 2011; Wang et al., 2013; Lee et al., 2019). Powell (2009) observed a strong positive correlation between the dry weight sediment concentrations of D4 with the sediment total OC content in Lake Pepin that created a spatial D4 concentration gradient across the lake. Lake Pepin is a wide stretch of the Mississippi River and therefore particles in the influent of the lake will settle based on size and density as the system transitions from lotic to lentic; upstream was shown to have larger solids containing a greater proportion of inorganics as compared to downstream, where smaller, more organic-rich particles fall out.

3.4.3 Terrestrial Environments

D4 is expected to be released to terrestrial environments via land application of biosolids and disposal of solid waste to landfills. With measured log K_{OC} values of 4.19–4.22 (Miller and Kozerski, 2007; Kozerski et al., 2014) and a water solubility of 0.056 mg/L (Dow Corning, 1991; Varaprath et al., 1996; NCBI, 2021), D4 will have a strong affinity for organic matter in terrestrial environments and leaching is not expected to occur.

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 Part 503) (U.S. EPA, 1993).

As discussed in Section 3.5.2, D4 is expected to be removed primarily by sorption to sludge in wastewater treatment, followed by air stripping. D4 removed by sorption to sewage sludge may be transferred to soil through biosolids amendment. D4 concentrations in sludge-applied soils may be lower than the biosolids themselves after the incorporation process due to dilution and abiotic processes such as hydrolysis and volatilization.

Studies measuring concentrations of D4 in sludge and biosolids from multiple countries outside the United States reported concentrations ranging from 0.04 to 46.5 µg/g dw (Kaj et al., 2005b; Schlabach et al., 2007; Zhang et al., 2011; Bletsou et al., 2013; Xu et al., 2013; Lee et al., 2014; Wang et al., 2015b; Li et al., 2016; Xu et al., 2016; COWI AS, 2018). In addition, Horii et al. (2019) reported D4 concentrations ranging from 0.17 to 0.56 µg/g ww from nine conventional WWTPs in Japan.

Data on D4 concentrations in biosolids resulting from non-industrial and industrial wastewater treatment in the United States were collected as part of the ECA (ERM, 2017a; SEHSC, 2021). D4 concentrations ranged from 0.448 to 6.16 µg/g dw in industrial sites and 0.055 to 0.659 µg/g dw in non-industrial sites. In addition, two studies reported D4 concentrations ranging from 0.2 to 1.77 µg/g dw in sludge samples from WWTPs located in the United States (Zhang, 2014) and Canada (Wang et al., 2015a). Biosolids with elevated D4 concentrations are to be expected at or near WWTPs that treat industrial waste.

With its water solubility (0.056 mg/L at 23 °C) (Dow Corning, 1991; Varaprath et al., 1996; NCBI, 2021) and affinity for sorption to organic matter in soil (log $K_{OC} = 4.19–4.22$ at 24.4–24.8 °C) (Miller and Kozerski, 2007; Kozerski et al., 2014), D4 is unlikely to migrate to groundwater and surface water via runoff after land application of biosolids (see Section 3.4.3.4). Furthermore, D4 is expected to dissipate in the soil via hydrolysis and volatilization processes (see Section 3.3.1.3).

3.4.3.2 Soil

When D4 is released to soil, approximately 90.5 percent of the mass fraction is estimated to partition to air (Table 3-4). A small percentage (9.5%) will remain in soil associated with solids and undergo abiotic degradation processes. The relative contributions of hydrolytic and volatilization processes to D4 dissipation from soil depend on the mineralogy of the soil and the percentage of relative humidity (soil moisture) (Xu and Chandra, 1999; Xu, 2007). D4 volatilization was observed to be predominant in moist soils, while acidic, drier, and clay heavy soils have shown to have greater hydrolysis rates (Buch and Ingebrigtson, 1979; Xu and Chandra, 1999). Refer to Section 3.3.1.3 for more information on hydrolysis.

As discussed in Section 3.3.1.3, DMSD is the main degradant product of D4 after undergoing hydrolysis in soil. DMSD is expected to degrade further in the environment to ultimately produce CO_2 and silicic acid (H_4O_4Si) and/or silica (SiO_2) (Figure 2-2) (Lehmann et al., 1994b; Chandra, 1997; ECHA, 2012).

3.4.3.3 Landfills

D4 is not listed under Subtitle C of the Resource Conservation and Recovery Act (RCRA) (40 CFR Part 261). No landfill leachate monitoring studies were identified during systematic review. D4 may be disposed into landfills through various waste streams such as consumer waste, residential waste, industrial waste, and municipal waste including dewatered wastewater biosolids. Because D4 is a highly volatile chemical with a Henry's law constant of 11.8 atm·m^3/mol at 21.7 °C (Xu and Kropscott, 2012, 2014), it is highly likely that D4 will be released to air from solid wastes.

The release of biogases from landfills is another point source of D4 emission to the air. Biogases are produced by biological decomposition of solid wastes in landfills (Schweigkofler and Niessner, 1999; McBean et al., 2002; Badjagbo et al., 2010; Gaj and Pakuluk, 2015; Rücker and Kümmerer, 2015). D4 will readily partition to the gaseous phase due to its water solubility (0.056 mg/L at 23 °C) and vapor pressure (0.9338 mm Hg at 25 °C) (Dewil et al., 2006; Surita and Tansel, 2014; NICNAS, 2020). Exceptionally high D4 concentrations were measured in biogas from landfills ranging from 0.196 to 29.1 mg/m^3 (Schweigkofler and Niessner, 1999; Badjagbo et al., 2009; Badjagbo et al., 2010; Piechota et al., 2013). Biogases can be captured and burned to generate renewable energy (heat or electricity) (Dewil et al., 2007; McBean et al., 2002; McBean, 2008; Badjagbo et al., 2009; Badjagbo et al., 2010), however not all waste disposal facilities do this, nor are they required to. If it is not captured and burned, D4 in the gaseous phase is expected to degrade slowly by reaction with •OH in the atmosphere (see Section 3.3.3.1), therefore D4 is likely to be persistent in outdoor air near release sites and undergo atmospheric long-range transport.

3.4.3.4 Groundwater

No groundwater monitoring studies were identified during systematic review. Given the strong affinity of D4 to adsorb to organic carbon (log K_{OC} = 4.19–4.22 at 24.4–24.8 °C) (Miller and Kozerski, 2007; Kozerski et al., 2014), D4 is expected to be immobile in soil and will not leach to groundwater. Furthermore, D4 migration to groundwater is unlikely due to its water solubility (0.056 mg/L at 23 °C) (Dow Corning, 1991; Varaprath et al., 1996; NCBI, 2021).

3.4.3.5 Key Sources of Uncertainty in the Assessment of Terrestrial Environments

PDMS is used in a broad range of industrial, medical, and consumer applications, therefore a significant amount of PDMS is used in down-the-drain products and released to the environment via wastewater effluent and sewage sludge (Chandra, 1997; Brooke et al., 2009c). All PDMS polymers contain residual amounts of cyclic siloxanes, including D4. The lower molecular weight (consisting lower viscosity) polymers may contain volatile cyclic siloxanes (<0.1–0.5%), and higher molecular weight (consisting higher viscosity) polymers may contain 1 to 3 percent volatile cyclic siloxanes (EC/HC, 2008c). Based on the information provided above, a small fraction of D4 may form during the breakdown of PDMS under certain conditions in landfills and soils where sewage sludge containing PDMS is applied (EC/HC, 2008c; Brooke et al., 2009c). However, the overall contribution of PDMS degradation is not significant and cannot be quantified based on the information reasonably available to the EPA.

3.5 Persistence Potential of D4

In the atmosphere, D4 is not expected to undergo significant direct photolysis in the atmosphere and will degrade slowly after reacting with photochemically produced •OH. D4 meets the criterion for persistence in the air compartment ($t_{1/2}$ > 2 days; 64 FR 60194, November 4, 1999) (Section 3.3.3.1). In surface water and sediment under environmentally relevant conditions, D4 is not expected to undergo biodegradation (Sections 3.3.2.1 and 3.3.2.2). The persistence of D4 in the surface water compartment is expected to be determined by hydrolysis. Given the range of empirical hydrolysis half-lives, D4 is not expected to be persistent ($t_{1/2}$ < 60 days) in the surface water compartment under environmentally relevant conditions (Section 3.3.1.1). As a hydrophobic chemical, D4 will be highly adsorptive to organic matter in suspended solids and sediment and is expected to be very persistent ($t_{1/2}$ > 180 days) (Sections 3.3.1.2 and 3.3.2.2). In soil under environmentally relevant conditions, D4 will undergo abiotic degradation such as hydrolysis and volatilization (Section 3.3.1.3). With a half-life of 126 hours (≈ 5.25 days), D4 is not expected to be persistent in the soil ($t_{1/2}$ < 180 days) (Section 3.2.2).

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).

Several assessments estimated that more than 99.9 percent of D4 disposed to municipal solid waste incineration will be mineralized (Lassen et al., 2005; Greve et al., 2014; ECHA, 2019; GSC, 2024). EPA identified an incineration study during systematic review. Horii et al. (2019) collected and analyzed dewatered sludge, incineration ash, and flue gas samples from nine sewage treatment plants (STPs) located in Saitama Prefecture, Japan. D4 concentration in incineration ash was found to be near the MDL (0.004 µg/g dw) and was two orders of magnitude lower than the mean D4 concentration in dewatered sludge (0.36 µg/g dw). The results indicate that D4 in dewatered sludge was effectively degraded by incineration (>99.9%) and D4 emission through incineration ash landfill was negligible. In conclusion, Horii et al. (2019) verified that incineration plants are not expected to be significant sources of D4 releases to the air.

On the other hand, D4 concentration in flue gas from the dewatered sludge incinerator was 0.17 µg/nm^3 (≈ 1.7×10^{26} µg/m^3). D4 present in flue gas will be released to the atmosphere where it is expected to degrade slowly by reaction with photochemically produced •OH) in the atmosphere.

3.5.2 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. After undergoing primary treatment, the wastewater undergoes a secondary treatment. Secondary treatment processes can remove up to 90 percent of the 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).

D4 is a volatile liquid with a vapor pressure of 0.9338 mm Hg at 25 °C (Lei et al., 2010), water solubility of 0.056 mg/L at 23 °C (Dow Corning, 1991; Varaprath et al., 1996; NCBI, 2021), log K_{OW} value of 6.488 at 25.1 °C (Kozerski and Shawl, 2007), and a Henry's law constant of 11.8 atm·m^3/mol at 21.7 °C (Xu and Kropscott, 2012, 2014). Based on these properties, the removal of D4 in activated sludge wastewater treatment is expected to be primarily by sorption to sludge and volatilization. Since D4 was not readily biodegradable under aerobic conditions based on two biodegradation tests (Bayer AG, 1995; Gledhill, 2005), biodegradation is not expected to be a significant removal process. The remaining D4 fraction sorbed to suspended solids in the wastewater treatment effluent may be discharged to receiving water (Wang et al., 2013; Zhang, 2014; Ha My Nu et al., 2021).

A total of 21 wastewater treatment studies were identified during systematic review. Two studies were rated as low-quality studies, another two as uninformative, and one as a medium-quality study. Those five studies were not selected for use in this risk evaluation. Out of the remaining 16 high-quality studies, only three studies reported the removal of D4 from wastewater in the United States and Canada using activated sludge treatment. Hydroqual (1993) reported a mean total D4 removal of approximately 88 percent from four activated sludge plants in New Jersey. Wang et al. (2013) reported a mean total removal of 98 percent from eleven wastewater treatment facilities in Canada. The study showed that the D4 removal rates were greater than 92 percent regardless of treatment type (*e.g.*, lagoon vs. secondary activated sludge vs. chemically-assisted primary). Wang et al. (2015a) reported a D4 removal efficiency of 96 percent in a secondary activated sludge WWTP located in Canada and approximately 29 percent of the removal was attributed to sorption to sludge. Sorption to sludge and volatilization in the aeration tank were identified as two of the main removal pathways for D4 in this study.

For comparison, the Sewage Treatment Plant model (STPWIN™) in EPI Suite™ (U.S. EPA, 2017) was run using the physical and chemical properties for D4 given in Table 2-1 (Figure 3-1). STPWIN™ in EPI Suite™ simulates a conventional WWTP that uses activated sludge secondary treatment. The biodegradation half-life parameter was set to 10,000 hours for the primary clarifier, aeration vessel, and settling tank, which is a default for non-biodegradable chemical. STPWIN™ calculated approximately 60 percent removal of D4 by adsorption to sludge and approximately 40 percent by volatilization with less than 1 percent removed by biodegradation and discharged to effluent, which verifies the results from monitoring studies.

The release of biogas from WWTPs is another point source of D4 emission to the air. Biogas consists of methane (CH_4) and CO_2 and is produced during anaerobic digestion of sewage sludge (Schweigkofler and Niessner, 1999; McBean et al., 2002; Badjagbo et al., 2010; Gaj and Pakuluk, 2015; Rücker and Kümmerer, 2015). Due to its Henry's law constant of 11.8 atm·m^3/mol at 21.7 °C (Xu and Kropscott, 2012, 2014), D4 will preferentially partition to the gaseous phase. Exceptionally high D4 concentrations were measured in biogas from STPs ranging from 0.5 to 10.1 mg/m^3 (Schweigkofler and Niessner, 1999; Piechota et al., 2013; Raich-Montiu et al., 2014). D4 in the gaseous phase is expected to degrade slowly by reaction with •OH in the atmosphere (see Section 3.3.3.1), therefore it will be persistent in the air near landfills and WWTPs.

3.6 Bioaccumulation Potential of D4

Information on bioconcentration and bioaccumulation in aquatic and terrestrial organisms is important to understanding the behavior of D4 in the environment and is a key component in assessing its risk to all living organisms, including humans.

3.6.1 Bioconcentration Factor

Bioconcentration is the uptake and retention of a chemical by an aquatic organism from ambient water only (U.S. EPA, 2003). Bioconcentration does not include chemical exposure through diet, but rather its uptake by respiratory and dermal surfaces (Arnot and Gobas, 2006). Bioconcentration factor (BCF) represents the tendency of a chemical to partition from water to an organism through the gills/respiratory route. BCFs are reliably measured from laboratory experiments where exposure dose can be controlled-, and steady-state conditions can be confirmed. BCF is traditionally calculated as the empirical ratio of biota-water concentrations at steady state, noted as BCF_{SS}. BCF may also be derived from the first-order uptake (k_1) and depuration (k_2 or k_T) kinetic rate constants, noted as BCF_k. Water concentrations should be analyzed such that the bioavailable (*i.e.*, dissolved) D4 fraction is captured, which can be difficult given D4's low water solubility and high volatility.

Considering the empirical evidence identified during systematic review, D4 is expected to bioconcentrate in fish species. Nine high-quality, non-guideline BCF studies reported D4 bioconcentration in aquatic biota (Table 3-1). Out of those nine studies, three studies reported aqueous exposure doses that were greater than D4's water solubility (Dow Corning, 1984; Springborn Laboratories, 1991d, e).[4] Since it is likely that these three studies did not capture the bioavailable D4 concentration in water, they were excluded for use in this risk evaluation.

Dow Corning (1992) conducted an 18-day exposure study with rainbow trout (*Oncorhynchus mykiss*) under flow-through conditions. From the water and fish concentrations provided in the study report, EPA calculated mean BCF values of 5,695 L/kg and 11,164 L/kg for 1-gram and 5-gram weight groups, respectively. Similarly, Dow Corning (1993a) conducted a 16-day exposure study with fathead minnow (*Pimephales promelas*) under flow-through conditions and reported a mean BCF value of 8,470 L/kg. However, the experimental design of both studies could not determine whether steady-state was achieved, which adds uncertainty to this data. Additionally, due to fish mortality in the Dow Corning (1992) study, the fish concentrations measured at later time points have small sample sizes, introducing some uncertainty.

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[4] Water solubility exceedance referring to the interstitial water concentration for both Springborn Laboratory studies listed in this sentence.

Fackler et al. (1995)[5] conducted a study consisting of a 28-day exposure period followed by a 14-day depuration period with fathead minnows (*Pimephales promelas*) under continuous flow-through conditions. The reported mean BCF_{SS} was 12,400 L/kg (95% CI: 9,380–16,100 L/kg), which was in close agreement with the reported BCF_k of 13,400 L/kg using the uptake and depuration rate constants of 2,450 per day and 0.183 per day, respectively. As the authors highlighted that the depuration concentration data did not fit a single compartment model, they also provided a BCF_k of 10,000 L/kg based solely on the uptake data. However, the BCF_k values are comparable regardless of the regression approach used.

Xue et al. (2020) reported BCF_{SS} and BCF_k values of 1,740 L/kg and 2,104 L/kg, respectively, in the muscle tissue of common carp (*Cyprinus carpio*) after 32 days of exposure to D4 at 4.79 ng/L followed by a 32-day depuration period. The BCF_{ss} value may be lower due to lack of steady state conditions as evidenced by the fish concentration uptake curve presented in the study. However, the reported BCF values were not lipid-normalized. In order to reduce any variability and uncertainty, EPA corrected the reported BCF values for lipid content using the study's average reported muscle tissue lipid content adjusted to wet weight percentages (11.9 ± 2.5% lipid, ww). The lipid-normalized BCF_{ss} and BCF_k values are 14,622 and 17,681 L/kg ww, respectively.

Kim et al. (2020) and Bernardo et al. (2022) discussed several issues with the experimental design of Xue et al. (2019, 2020) that may have a negative impact on the resulting BCF data. First, the fish length ranged from 11.1 to 15.6 cm and only four fish were within the recommended 8 ± 4 cm range (OECD, 2012), which may indicate that the fish were at different developmental stages. Secondly, fish were acclimated for seven days, which is significantly shorter than the recommended 14 days (OECD, 2012). Lastly, the fish were not fed throughout the experiment as recommended (OECD, 2012), and a significant decrease in fish body weights may have distorted the uptake, elimination, and metabolic responses of the fish. Kim et al. (2020) noted additional errors in the results from Xue et al. (2019): first, the reported BCF values were in wet-weight basis, however the concentrations used to calculate the BCF values were on dry-weight basis; and second, the exposure and depuration regressions from which k_1 and k_2 were derived did not fit the biota concentration values well, therefore yielding erroneous kinetic parameters. Upon adjusting for these errors, Kim et al. (2020) calculated a BCF_k value of 1,673 L/kg ww using optimized k_1 and k_2 values. The lipid-normalized BCF_k value is 14,059 L/kg ww.

Two dietary studies reported D4 BCFs that were determined semi-empirically using the ADME-B model described in Gobas et al. (2019) (described further in Appendix B.2). Compton (2019) conducted a study similar to OECD TG 305-III (OECD, 2012), which consisted of a 10-day exposure period followed by a 28-day depuration period with juvenile rainbow trout (*Oncorhynchus mykiss*). The reported BCF value (± standard error of the mean [SE]) was 2,865 (± 1,112 SE) L/kg. Using the same method, Cantu et al. (2024) reported a BCF value of 4,153 (± 534 SE) L/kg and 8,258 (± 1,062 SE) L/kg with aqueous DOC concentrations of 2.0 and 7.1 mg-OC/L, respectively. Cantu et al. (2024) noted the sensitivity of BCF to variations in aqueous DOC and this indicates the importance of D4 sorption to dissolved organic matter in water. The relationship between aqueous DOC concentration and D4 BCF is further discussed in Appendix B.2. Both semi-empirical BCF values derived using the ADME-B model agree well with the empirical BCF values (Figure 3-5).

In order to determine a representative, central tendency BCF value for D4, EPA accounted for the

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[5] Springborn Laboratories (1991a, 1991b) is the same study as Fackler et al. (1995). Therefore, both studies will not be discussed in risk evaluation.

varying lipid contents of the fish species represented in the dataset. Briefly, EPA first averaged the lipid-normalized BCFs from the four empirical laboratory BCF studies (Dow Corning, 1992, 1993a; Fackler et al., 1995; Xue et al., 2020), then applied the recommended generic lipid content of 5 percent (OECD, 2012) to obtain a BCF of 8,795 L/kg. See Appendix B.2 for more information.

3.6.2 Bioaccumulation Factor

While laboratory derived BCF values are important for isolating uptake rates from the respiratory route, field-derived bioaccumulation factors (BAFs) tend to be more representative of environmentally relevant accumulation dynamics. BAFs represent the extent to which a chemical is absorbed by biota from dietary and environmental (respiratory and dermal) exposure routes determined at steady state. Because of this, BAFs of hydrophobic chemicals are often expected to be greater than respective BCFs that capture respiratory uptake from the environment only. However, for chemicals such as D4 that undergo biotransformation in the gastrointestinal tract (thus exhibiting low uptake rates from dietary routes), the magnitudes of BAFs and BCFs may be comparable (Gobas et al., 2019; Cantu et al., 2024). Similar to BCFs, BAFs may be determined empirically by the ratio of chemical concentration in biota to the concentration of freely dissolved chemical in water (BAF_{ss}) or from empirically-derived kinetic rates (BAF_k).

Two high-quality field studies characterizing D4 BAF in crucian carp (*Carassius carassius*) in freshwater were identified during systematic review. Guo et al. (2021) reported a non-lipid-normalized mean BAF value of 5,900 L/kg in the muscle of crucian carp collected from seven sites in a river near a methyl siloxane production factory in Liaoning Province, northeast China. A lipid-normalized BAF could not be calculated since the study did not provide the lipid content of the fish samples. In addition, the aqueous D4 concentrations from three out of seven sites were below the method detection limit (<1.5 ng/L) while measured D4 concentrations in carp were all quantifiable, which adds an uncertainty in the reported BAF value. Wang et al. (2021) reported a lipid-normalized mean BAF value of 4,141 L/kg ww in the muscle of crucian carp collected from three major rivers in South Korea. Wang et al. (2021) assumed a carp muscle lipid content of 1.67 percent, which then was used to back calculate a non-lipid corrected BAF. The non-lipid-normalized BAF is 69 L/kg, which is much smaller than the field-derived BAF obtained for *Carassius carassius* by Guo et al. (2021). The measured aqueous concentrations of D4 in Wang et al. (2021) ranged from not-detects (n.d.) to 271 ng/L with a median of 52.7 ng/L, and the biota concentrations ranged from n.d. to 31 ng/g ww with a median of 0.656 ng/g ww. The measured aqueous concentrations of D4 in Guo et al. (2021) ranged from less than 1.2 to 3.2 ng/L with a mean of 2 ng/L, and the biota concentrations ranged from 6.5 to 18 ng/g ww with a mean of 13 ng/g ww. One possible reason the aqueous D4 concentrations in Wang et al. (2021) were inflated compared to those from Guo et al. (2021) is because the water samples in Wang et al. (2021) were not filtered and included both dissolved and particulate-bound D4 fractions in the BAF ratio. However, it is unclear if Guo et al. (2021) captured losses to the filtration apparatus during extraction recovery analyses. Moreover, as highlighted by Cantu et al. (2024) and discussed in Appendix B.2, differences in aqueous DOC concentration can greatly influence respiratory uptake rates and thus contribute to variation in BAFs. Additionally, Wang et al. (2021) did not report how non-detects were handled, which may also greatly influence the final reported values. Because no additional data characteristics were provided (*e.g.*, whether samples were location-matched, or the carp concentrations were only given for muscle tissue measurements), it is difficult to further contextualize this discrepancy in BAF magnitude. Figure 3-5 summarizes the high-quality BCF and BAF values identified for D4, illustrating the relatively wide range of available values.

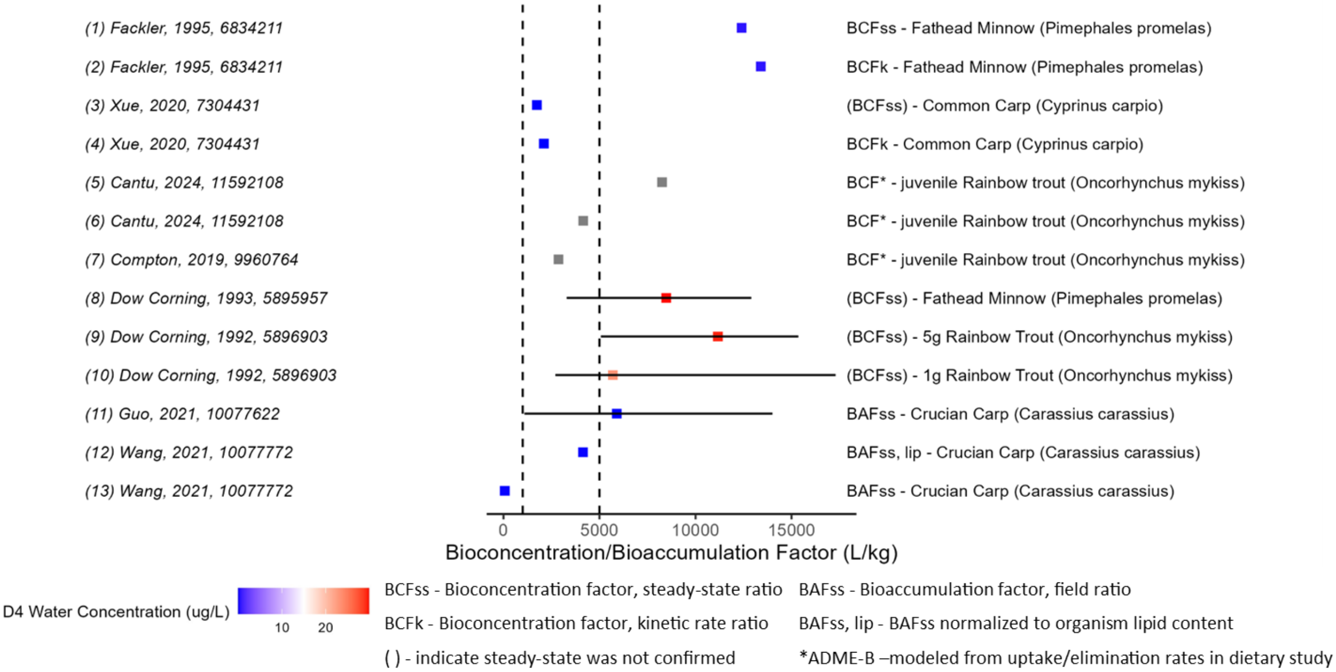

Figure 3-5. Summary of High-Quality Identified Bioconcentration and Bioaccumulation Factors
Whiskers illustrate BCF/BAF ranges where available. Grey markers indicate feeding studies, therefore water concentrations were not relevant. Dashed lines indicate "bioaccumulative" thresholds of 1,000 and 5,000 L/kg (U.S. EPA, 2012).

3.6.3 Biota-Sediment Accumulation Factor

A biota-sediment accumulation factor (BSAF) captures accumulation to biota from the sediment compartment. This is expected to be central to D4 uptake by biota since D4 is expected to sorb to organics that settle in the sediment compartment. Bioaccumulation is implied when a BSAF is (significantly) greater than one. However, a generic, theoretical BSAF value of 1.7 was estimated based on partitioning of non-ionic organic compounds between tissue lipids and sediment carbon (ASTM, 1997). A BSAF value less than 1.7 indicates less partitioning of an organic compound into lipids, whereas a BSAF value greater than 1.7 indicates a greater uptake of the compound (Ozkoc et al., 2007; Hong et al., 2014; Zhi et al., 2019; Bernardo et al., 2022). BSAF values are most relevant to informing accumulation in benthic-dwelling species (*e.g.*, mussels, crustaceans) rather than fish species present in the water column. Because of this, only studies reporting BSAF values for benthic-dwelling, non-fish organisms are reported in Table 3-1. Nonetheless, several fish species (*e.g.*, fat greenling, crucian carp) feed on material in the benthos and may ingest D4 from incidental sediment ingestion.

Nine high-quality studies reporting BSAF data were identified during systematic review. The study by Horii et al. (2013) was excluded from use in this risk evaluation because all sediment concentrations were below the MDL of the study, which decreased confidence in the precision of the reported BSAF values as compared to the other eight high-quality studies.

Six studies reported BSAF values for benthic dwelling organisms. Evonik Goldschmidt (2009) reported mean BSAF values of 1.2 g-OC/g-lipid for shrimp from the inner Oslofjord and 2.6 g-OC/g-lipid for shrimp from the outer Oslofjord, Norway. Similar to other aquatic monitoring studies (see Section 3.4.2), the authors reported overall greater concentrations of D4 in water, sediment, and biota samples collected in the more densely populated inner fjord area as compared to in the outer fjord that sits further from human development. Zhi et al. (2019) examined D4 BSAFs in three mollusk species (*Mytilus galloprovinvialis*, *Cyclina sinensis*, and *Crassostrea talienwhanensis*) collected from the Bohai Sea, China. The reported mean BSAF was 0.42 ± 0.06 g-OC/g-lipid (soft tissue). Springborn Laboratories (1991d, 1991e) conducted a series of 14-day definitive toxicity studies to determine the effect of sediment organic carbon concentrations on the bioaccumulation of 10-day old, second instar midge larvae (*Chironomus tentans*). The studies were conducted under flow-through conditions at five D4 concentrations and three organic carbon contents. BSAF values were obtained from day 14 measurements from treatments in which survival rates between treatment and control vessels were not statistically different. The reported mean BSAF values were 2.15 ± 1.57, 1.25 ± 0.21, and 0.81 ± 0.27 in sediment with low (0.23%), medium (2.3%), and high (3.9–4.1%) organic carbon content, respectively. Using the same test method and organism, Kent et al. (1994) reported mean BSAF values of 2.15 ± 0.64, 1.3 ± 0.00, and 0.7 ± 0.08 in sediment with low (0.23%), medium (2.3%), and high (4.1%) organic carbon content, respectively. However, these values were not OC- or lipid-normalized and therefore cannot be compared to the other normalized BSAF values presented in this section. Powell et al. (2009) reported BSAFs in eighteen different species that were collected from Lake Pepin, Minnesota. Only three species had a sample size that was equal to or greater than four ($n \geq 4$). The mean BSAF values were 19.2 for midge larvae (*Chironomus* sp.), 2.6 for adult gizzard shad (*Dorosoma cepedianum*), and 2.1 for emerald shiner (*Notropis atherinoides*). All BSAF values reported by Powell et al. (2009) are based on whole organism concentrations. While there is considerable uncertainty in the BSAF values due to lack of field blanks, small samples sizes, low sediment concentrations (background-corrected D4 < MDL), and the use of uncensored values), it may be possible for D4 to accumulate more readily in benthic organisms that feed on sediment-dwelling invertebrates and organic material as compared to species at higher trophic levels (Powell et al., 2009).

The remaining three studies reported BSAF values for fish only. It should be noted that the sample sizes for several species in the studies reporting fish BSAFs are quite low (*i.e.*, ≤ 11 individuals). Hong et al. (2014) reported a mean BSAF value of 0.716 ± 0.456 (whole organism) kg-OC/kg-lipid for fat greenling (*Hexagrammos otakii*; n = 6) collected from the Dalian Sea, China. Krogseth et al. (2017) reported BSAF values of 3.4 ± 1.9 (muscle tissue) and 1.5 ± 1.1 (whole organism) g-OC/g-lipid for arctic char (*Salvelinus alpinus*; n = 11) and sticklebacks (*Gasterosteus aculeatus*; n = 6), respectively, collected from Lake Storvannet, Norway. Wang et al. (2021) reported a mean BSAF of 2.36 ± 1.84 (muscle tissue) g-OC/g-lipid in crucian carp (*Carassius carassius*; n = 106) collected from three South Korean river basins.

Empirically-determined BSAF values for D4 fall on both sides of the 1.7 threshold, indicating that D4 may accumulate to biota from the sediment in some environments.

3.6.4 Biomagnification Factor

Biomagnification factor (BMF) represents the tendency of a chemical to increase in concentration from prey to predator. Like with BCF and BAF, BMF can be derived either as an empirical ratio of the concentration of chemical in the predator to the concentration of the chemical in the predator's diet at steady state (BMF_{ss}), or as determined from kinetic constants from dietary uptake and depuration studies (BMF_k). Especially for lipophilic chemicals, it may be appropriate for BMF to be calculated based on lipid-normalized chemical concentrations in both the diet (prey) and consumer (predator) (*i.e.*, BMF_L), as lipid content may differ among trophic levels. A BMF value greater than 1 indicates the occurrence of biomagnification.

While BMF may be estimated from field measurements, controlled laboratory experiments allow for the following conditions of an accurate BMF determination to be confirmed: that steady state is reached, that diet is the sole source of exposure to the predator, and that a consistent chemical dose to the predator is maintained. These are important variables to control for when characterizing uptake and depuration kinetics from dietary exposures. For this reason, field-derived BMF values from Dow Corning (2009), Powell et al. (2010), Dow Corning (2010), and Xue et al. (2019) were excluded from use in this risk evaluation.

Three high-quality studies used OECD TG 305 (OECD, 2012) to carry out laboratory dietary biomagnification tests, with modifications. Woodburn et al. (2013) measured BMF in rainbow trout (*Oncorhynchus mykiss*) and obtained a lipid-normalized, steady-state mean $BMF_{L,ss}$ value of 0.66 ± 0.06. The ratio of k_1/k_2 yielded greater BMF_k values of 1.7 ± 0.5 and 4.0 ± 1.2 measured from ww and lipid-normalized ww, respectively. These values are likely conservative estimates due to assumptions and uncertainties in the two-compartment model used to obtain k_1 and k_2 that decreased the value of k_2. Compton (2019) reported a similar result with a BMF_L value of 0.35 ± 0.21 (whole body minus gut) for juvenile rainbow trout in a dietary exposure study, using Equation 3-1. Using the same method, Cantu et al. (2024) reported a BMF_L value of 0.444 ± 0.079 (SE).

Equation 3-1

$$BMF_L = \frac{E_{Diet} \times F}{k_{BT}} \times \frac{\varphi_{L,Diet}}{\varphi_{L,Fish}}$$

Where:

BMF_L = Lipid-normalized biomagnification factor (kg/kg)
E_{Diet} = Dietary uptake coefficient (unitless)
F = Proportional feeding rate (kg-food/kg-ww fish)
k_{BT} = Depuration rate constant (d^{-1})
$\varphi_{L,Diet}$ = Lipid content of diet (kg-lipid/kg-food)
$\varphi_{L,Fish}$ = Lipid content of fish (kg-lipid/kg-fish)

The BMF values from three high-quality laboratory studies were below 1, which indicates that D4 is unlikely to biomagnify.

3.6.5 Trophic Magnification Factor

Trophic magnification occurs when the average biological body burden of a chemical increases with trophic level within a food web. It is often estimated using a trophic magnification factor (TMF). A TMF value greater than one indicates trophic magnification within a food web, whereas a TMF less than one indicates trophic dilution. When trophic dilution occurs, the concentration of a pollutant decreases as the trophic level increases. It could be the result of a net balance of ingestion rate, uptake from food, internal transformation, or elimination processes favoring loss of pollutant that enters the organism via food.

Eight high-quality studies estimating the TMF of D4 were identified during systematic review. These studies represent a range of habitat types, locations, and different types and sizes of food webs. All but two studies reported multiple TMF estimates by including multiple food web configurations, calculation methods, and/or sublocations. For instance, five studies employed and reported results of both ordinary least-squares (OLS) regressions and bootstrapped regressions. Therefore, the entire dataset comprises of 24 individual TMF estimates. Of these, five reported TMF values were greater than 1.

Three TMF studies were conducted in China, in bodies of water experiencing both point and non-point sources of D4 exposure. Cui et al. (2019) found D4 likely to biomagnify in a mixed, marine food web comprising eighteen species in the Bohai Sea in northern China; the obtained TMF was 1.7 (95% CI: 1.1–2.6). Additionally, the authors used two benchmark chemicals known to biomagnify, BDE-47 and BDE-99, to confirm that the study design was able to capture magnification (100% probability of obtaining TMF > 1 was determined for both reference compounds).

Similarly, Jia et al. (2015) reported trophic magnification in a mixed, marine food web of Dalian Bay, China. Five fish, one crustacean, five mollusk, and one polychaete species, as well as sea lettuce were included in the analysis, totaling of 305 samples. The OLS yielded a TMF estimate of 1.16 (95% CI: 0.94–1.44), while the bootstrapped regression yielded a TMF of 1.5 (95% CI: 1.2–1.8). Again, the authors confirmed the representativeness of their study design with the benchmark chemical BDE-99, yielding a probability of 99.7 percent of obtaining a TMF greater than 1.

To contrast, He et al. (2021) reported likely trophic dilution (bootstrapped TMF = 0.75; 95% CI: 0.58–1.93) among twelve fish species from a freshwater food web in Lake Chaohu, China. Similarly, Kim et al. (2022) reported an OLS-derived TMF value of 0.9 from fifteen fish species in the Geum River, South Korea. He et al. (2021) used a markedly smaller sample size (<50) than Jia et al. (2015) and Cui et al. (2019), likely contributing to the relatively larger variance in the obtained probability distribution for TMF. Additionally, He et al. (2021) was the only study to use dry weight, lipid-normalized concentrations in their analysis while others used lipid-normalized wet weights.

Trophic dilution of D4 was also reported in a pelagic marine food web in Tokyo Bay, a largely eutrophic bay in Japan (Powell et al., 2017). The OLS regression across these fish species yielded a TMF of 1.3, though with a relatively large variance range (95% CI: 0.5–3.3), likely due to the small sample size of 21. The bootstrapped regression was much more precise, yielding a median TMF of 0.6 with 95% CI: 0.5–0.8. Powell et al. (2017) also reported a combined TMF range of 2.2 to 2.7 from the co-measured benchmark chemicals CB-180 and CB-153.

Two studies found D4 to exhibit trophic dilution in both marine and freshwater ecosystems in Norway. Borgå et al. (2013) investigated several configurations of pelagic, freshwater food webs in Lake Mjøsa and Lake Randsfjord including brown trout (*Salmo trutta*), smelt (*Osmerus eperlanus*), vendace (*Coregonus albula*), whitefish, zooplankton (*Mysis relicta*), among other epi- and hypolimnetic species. Using OLS regression, Borgå et al. (2013) found mean TMF values from 0.57–0.76 across five food web scenarios. Additionally, the reported benchmark chemicals, dichlorodiphenyldichloroethylene (p,p′-DDE), polychlorinated biphenyls (PCBs), and polybrominated diphenyl ethers (PBDEs), exhibited a TMF range from 1.41–5.72, strengthening confidence in the D4 trophic dilution conclusion. Powell et al. (2018) found D4 to exhibit trophic dilution in Oslofjord across all of four food web configurations representing both demersal and pelagic systems. Mean OLS-derived TMFs ranged from 0.5–0.7 and median bootstrapped values ranged from 0.4–0.7, however samples in this study were not analyzed for a benchmark compound.

Two studies conducted in Lake Pepin and Lake Erie both reported trophic dilution to be likely in each of the sampled food webs. Powell et al. (2009) calculated the TMF from 2 benthic macroinvertebrates and 15 fish species in Lake Pepin. With the OLS regression method, a TMF of 0.8 (95% CI: 0.6–1.1) was obtained, and the bootstrapped regression yielded a TMF of 0.5 (95% CI: 0.3–0.7). Similarly, McGoldrick et al. (2014) obtained a bootstrapped TMF of 0.74 (95% CI: 0.39–1.2) from seven fish species and one invertebrate species collected from the Western Basin of Lake Erie.

It is important to note that even those studies reporting TMF values greater than one obtained TMF ranges relatively close to one as compared to reference chemicals whose TMF values range from 1.2 to 5.72 (Borgå et al., 2013; McGoldrick et al., 2014; Jia et al., 2015; Powell et al., 2017). This fact combined with the remainder of the dataset shows overall low potential for D4 to exhibit trophic magnification across several ecosystem and food web configurations. While there may be specific instances of biomagnification in certain food webs and in certain predator-prey relationships, especially in lower trophic levels and sediment-dwelling organisms, the majority of the empirical evidence gathered from high-quality data suggests low potential for biomagnification of D4.

3.6.6 Key Sources of Uncertainty in the Assessment of Bioaccumulation Potential

Many sources of uncertainty in bioaccumulation assessments result from study design. For example, water samples for BCF and BAF studies should be analyzed such that the bioavailable (*i.e.*, dissolved) fraction is captured. This can be difficult for volatile, hydrophobic chemicals with low solubilities like D4, as discussed in Section 3.4.2.3. Additionally, Cantu et al. (2024) highlighted how D4 uptake via gill respiration, and thus BCF, is greatly influenced by DOC concentration of the aqueous environment (see Appendix B.2).

There are differing sources of uncertainty associated with field-derived BAF, BMF, BSAF and TMF values as compared to laboratory-derived bioaccumulation metrics. Field studies introduce more uncertainty than laboratory studies, specifically when no field controls are collected, small sample sizes, the inability to confirm steady-state conditions, and uncertainties surrounding diet and additional exposure routes (Dow Corning, 2009; Powell et al., 2009; Xue et al., 2019). Additional sources of uncertainty include low detection and quantification frequencies in sampled biota (Borgå et al., 2013; Powell et al., 2018), and relatively small sample sizes (Borgå et al., 2013; McGoldrick et al., 2014; Powell et al., 2018; Kim et al., 2022), both of which can skew accumulation assessments if not taken into consideration. Nonetheless, field measurements sometimes provide a more representative picture of accumulation dynamics in natural environments when compared to engineered laboratory settings. As laboratory experiments have better control over routes of exposure, these studies are important to inform the impact of exposure characteristics (*e.g.*, dietary vs. respiration, controlled chemical concentration and exposure times) on chemical uptake and depuration. Because of this, both laboratory- and field-measured bioaccumulation metrics were considered in the overall analysis of the bioaccumulation potential of D4.

3.7 Weight of Scientific Evidence Conclusions for Fate and Transport Assessment

The weight of scientific evidence supporting the fate and transport assessment is based on the strengths, limitations, and uncertainties associated with the fate and transport studies evaluated within and outside systematic review. The judgment is summarized below using confidence descriptors: robust, moderate, slight, or indeterminate. This approach is consistent with the 2021 Draft Systematic Review Protocol (U.S. EPA, 2021d).

3.7.1 Strengths, Limitations, Assumptions, and Key Sources

Given the consistent results from numerous high-quality studies, there is a robust confidence that D4:

- is expected to undergo rapid hydrolysis in surface water and its hydrolysis rate is dependent on the pH and temperature (Section 3.3.1.1);
- does not undergo biodegradation in water under aerobic conditions (Section 3.3.2.1);
- does not undergo biodegradation in sediment under aerobic and anaerobic conditions and will have a strong affinity for organic carbon (Section 3.3.2.2);
- is not expected to undergo significant direct photolysis and will degrade slowly by reaction with

photochemically produced hydroxyl radicals (•OH) in the atmosphere (Section 3.3.3.1);

- is not expected to undergo photolysis in aquatic environments under environmentally relevant conditions since it does not absorb wavelengths greater than 290 nm (Section 3.3.3.2);
- has the potential to undergo atmospheric long-range transport due to its persistence in the air (Section 3.4.1.1);
- is expected to volatilize from surface water (Section 3.4.2.1);
- is likely to volatilize from moist soils and undergo hydrolysis in drier, acidic soils with higher clay content (Sections 3.3.1.3 and 3.4.3.2);
- is expected to transform into DMSD and its oligomer silanols in water, soil, and sediment (Section 3.3.1);
- will be effectively degraded (>99.9%) and its emission through incineration ash landfill will be negligible (Section 3.5.1);
- will be removed significantly after undergoing wastewater treatment primarily by sorption to sludge and volatilization, with a small fraction of D4 in the wastewater effluent being discharged to receiving water (Section 3.5.2);
- is likely to bioconcentrate and bioaccumulate in fish (Sections 3.6.1 and 3.6.2);
- may accumulate in sediment-dwelling organisms (Section 3.6.3); and
- is not expected to biomagnify in predator-prey relationships (Section 3.6.4).

As a result of varied conclusions, there is a moderate confidence that D4:

- does not exhibit trophic magnification (Section 3.6.5).

Findings with a robust weight of evidence had two or more high-quality studies that were largely in agreement with each other. Findings that have a moderate weight of evidence were based on high-quality studies that were mostly in agreement but varied in sample size and consistency of results. Due to D4's water solubility and volatility, certain physical and chemical properties may be difficult to measure experimentally, such as water solubility and partitioning coefficients (*e.g.*, K_{OW}, K_{OA}, K_{AW}) with standard guideline tests (Varaprath et al., 1996; Xu and Kropscott, 2012; Xu et al., 2014; Xu and Kropscott, 2014). The selection of these values was based on consideration of all reasonably available information and used professional judgment which incorporated consideration of the overall data quality ranking of the references.

4 PHYSICAL CHEMISTRY AND FATE AND TRANSPORT ASSESSMENTS CONCLUSIONS

D4 is found in various environmental media including air, water, sediment, soil and biota due to its widespread production and application. The physical and chemical properties of D4 determine its environmental fate and transport behavior, which is important in understanding D4's persistence in the environment and its potential for bioaccumulation, while considering transport, partitioning, and removal pathways. Based on D4's water solubility (0.056 mg/L 23 °C), Henry's law constant (11.8 $\text{atm}\cdot\text{m}^3/\text{mol}$ at 21.7 °C), and log K_{OC} values (4.19–4.22 at 24.4–24.8 °C), D4 will preferentially partition to organic carbon, which suggests that the major environmental compartments will be air, soil, biosolids, and sediment. Based on these properties, the removal of D4 in wastewater treatment processes is expected to be primarily by sorption to sludge, followed by volatilization. Surface water is highly likely to be a minor pathway, and the main sources of D4 are from wastewater effluents and down-the-drain disposals from industrial and consumer uses. Hydrolysis is the dominant pathway for D4 degradation in surface water and its hydrolysis rate is highly dependent on pH and temperature. D4 may undergo volatilization under specific environmental conditions. A fraction of D4 can be transported to sediments from overlying surface water via advection, dispersion, and sorption to suspended solids that can settle out from the water column. In areas where continuous releases of D4 take place, higher D4 concentrations in surface water can be expected. This also applies to suspended and benthic sediments. D4 does not undergo biodegradation in water under aerobic conditions and in sediment under both aerobic and anaerobic conditions. Since D4 is expected to be removed primarily by sorption to sludge in wastewater treatment, it may be transferred to soil via land application of biosolids. Due to its water solubility and strong affinity for organic carbon, D4 is unlikely to migrate to groundwater, surface water, or be uptaken by crops and plants. Instead, D4 is expected to dissipate in the soil via abiotic processes such as hydrolysis and volatilization.

When released directly to the atmosphere, D4 is not expected to undergo significant direct photolysis and will degrade slowly after reacting with photochemically produced ·OH. Due to its persistence in the atmosphere ($t_{1/2}$ > 2 days), D4 has the potential to undergo atmospheric long-range transport. However, D4 is not expected to undergo wet or dry deposition due to its low water solubility and high vapor pressure. Atmospheric D4 concentrations may be elevated in close proximity to the release of biogases from landfills and aeration tanks in WWTPs due to its volatility (0.9338 mm Hg at 25 °C). Under indoor settings, D4 air concentrations were observed to be significantly higher than those from outdoor air and are strongly correlated with occupant density. D4 was also detected in indoor dust, but due to its volatility, higher D4 air concentrations are found in the gaseous phase.

Overall, D4 is not expected to be persistent in water and soil under environmentally relevant conditions but will be persistent in air and sediments. However, it may be continually present in water where there is continuous release of D4. In the environment, D4 is expected to transform into silanols and DMSD. For biota, D4 is highly likely to bioconcentrate and bioaccumulate in fish. In addition, D4 may accumulate in sediment-dwelling organisms. Though D4 can, in some instances, biomagnify and exhibit trophic magnification, the weight of scientific evidence suggests that D4 is generally not expected to biomagnify in predator-prey relationships or exhibit trophic magnification.

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APPENDICES

Appendix A D4 DEGRADANTS

A.1 Physical and Chemistry Assessment

A.1.1 Approach and Methodology

EPA gathered and evaluated physical and chemical property data and information according to the process described in the *Draft Systematic Review Protocol Supporting TSCA Risk Evaluations for Chemical Substances* (U.S. EPA, 2021d) (also referred to as the “2021 Draft Systematic Review Protocol”). During the data evaluation for D4’s degradants, EPA considered both measured and estimated physical and chemical property data/information summarized in Table_Apx A-1, Table_Apx A-2, Table_Apx A-3, and Table_Apx A-4 as applicable. Information on the full, extracted dataset is available and provided in the supplemental file, *Draft Data Quality Evaluation and Data Extraction Information for Physical and Chemical Properties for Octamethylcyclotetrasiloxane (D4)* (U.S. EPA, 2025d).

A.1.2 Final Selected Physical and Chemical Properties

For some physical and chemical properties, there are multiple high-quality values available for selection that were identified during systematic review. The majority of selected data were collected under standard environmental conditions (*i.e.*, 20–25 °C and 760 mm Hg). However, some properties are reported at several experimental temperatures to provide additional context to how D4 behaves under environmentally relevant temperatures in real world scenarios. This is especially important for providing foundational context for environmental fate and transport endpoints (*i.e.*, biodegradation rates, wastewater removal efficiency, bioaccumulation factors, etc.) as they demonstrate the variety of environmental conditions where D4 may be measured.

Table_Apx A-1. Physical and Chemical Properties of Dimethylsilanediol (DMSD)

Property	Selected Value[a]	Reference(s)	Data Quality Rating[b]
Molecular formula	$C_2H_8O_2Si$	Elsevier (2021a)	High
Molecular weight	92.17 g/mol	Elsevier (2021a)	High
Physical form	Crystal phase – interplanar spacing and leafs	Elsevier (2021c)	High
Melting point	98.8 ± 1.56 °C	Elsevier (2021c)	High
Boiling point	No data identified		
Density	1.095–1.099 g/cm^3	Elsevier (2021c)	High
Vapor pressure	No data identified		
Vapor density	No data identified		
Water solubility	2.45E06 mg/L at 25 °C	Elsevier (2021c)	High
Octanol/water partition coefficient (log K_{OW})	–0.41 ± 0.1 at 20.1 °C	Xu and Kropscott (2012) as cited in Elsevier (2021c)	High
Octanol/air partition coefficient (log K_{OA})	6.40 ± 0.31 at 20.1 °C	Xu and Kropscott (2012)	High
Henry's law constant	3.48E–09 atm·m^3/mol at 20.1 °C	Xu and Kropscott (2012)	High
Flash point	No data identified		
Autoflammability	No data identified		
Viscosity	No data identified		
Refractive index	1.444–1.456 at 25 °C	Elsevier (2021c)	High
Dielectric constant	No data identified		

[a] Measured unless otherwise noted

[b] "Data Quality Rating" apply to all references listed in this table

Table_Apx A-2. Physical and Chemical Properties of Tetramethyldisiloxanediol (Dimer Diol)

Property	Selected Value[a]	Reference(s)	Data Quality Rating[b]
Molecular formula	$C_4H_{14}O_3Si_2$	Elsevier (2021a)	High
Molecular weight	166.33 g/mol	Elsevier (2021a)	High
Physical form	Needle-shaped, monoclinic, white crystal	Elsevier (2021d)	High
Melting point	66 °C	Haynes (2014a); Elsevier (2021d)	High
Boiling point	No data identified		
Density	1.095 g/cm^3 at 25 °C	Haynes (2014a)	High
Vapor pressure	No data identified		
Vapor density	No data identified		
Water solubility	110,000–115,000 mg/L at 20–25°C	Elsevier (2021d)	High
Octanol/water partition coefficient (log K_{OW})	0.926 ± 0.035 at 12°C 0.962 ± 0.049 at 20°C 1.036 ± 0.042 at 27°C 1.099 ± 0.025 at 35°C	Dow Chemical (2022b)	High
Octanol/air partition coefficient (log K_{OA})	No data identified		
Henry's law constant	2.58E–07 atm·m^3/mol at 12 °C 5.25E–07 atm·m^3/mol at 20 °C 1.73E–07 atm·m^3/mol at 27 °C 1.39E–07 atm·m^3/mol at 35 °C	Dow Chemical (2022b)	High
Flash point	No data identified		
Autoflammability	No data identified		
Viscosity	No data identified		
Refractive index	1.457–1.466 at 25 °C	Elsevier (2021d)	High
Dielectric constant	No data identified		

[a] Measured unless otherwise noted

[b] "Data Quality Rating" apply to all references listed in this table

Table_Apx A-3. Physical and Chemical Properties of Hexamethyltrisiloxanediol (Trimer Diol)

Property	Selected Value[a]	Reference(s)	Data Quality Rating[b]
Molecular formula	$C_6H_{20}O_4Si_3$	Elsevier (2021a)	High
Molecular weight	240.48 g/mol	Elsevier (2021a)	High
Physical form	No data identified		
Melting point	–23 to –1.9 °C	Elsevier (2021a)	High
Boiling point	72–74 °C at 0.3 torr 79–91 °C at 2–3 torr 106 °C at 6 torr	Elsevier (2021a)	High
Density	0.991–1.0127 g/cm^3 at 20–25 °C	Elsevier (2021a)	High
Vapor pressure	No data identified		
Vapor density	No data identified		
Water solubility	No data identified		
Octanol/water partition coefficient (log K_{OW})	2.125 ± 0.249 at 12 °C 2.369 ± 0.104 at 20 °C 2.391 ± 0.112 at 27 °C 2.512 ± 0.165 at 35 °C	Dow Chemical (2022b)	High
Octanol/air partition coefficient (log K_{OA})	No data identified		
Henry's law constant	1.12E–06 atm·m^3/mol at 12 °C 1.23E–06 atm·m^3/mol at 20 °C 1.13E–06 atm·m^3/mol at 27 °C 1.37E–06 atm·m^3/mol at 35 °C	Dow Chemical (2022b)	High
Flash point	No data identified		
Autoflammability	No data identified		
Viscosity	No data identified		
Refractive index	1.405–1.409 at 20–25 °C	Elsevier (2021a)	High
Dielectric constant	No data identified		

[a] Measured unless otherwise noted
[b] "Data Quality Rating" apply to all references listed in this table

Table_Apx A-4. Physical and Chemical Properties of Octamethyltetrasiloxanediol (Tetramer Diol)

Property	Selected Value[a]	Reference(s)	Data Quality Rating[b]
Molecular formula	$C_8H_{26}O_5Si_4$	Elsevier (2021a)	High
Molecular weight	314.64 g/mol	Elsevier (2021a)	High
Physical form	No data identified		
Melting point	–5 °C	Elsevier (2021b)	High
Boiling point	86–88 °C at 0.4 torr 97–100 °C at 2 torr	Elsevier (2021b)	High
Density	0.9881–0.9886 g/cm^3 at 20 °C	Elsevier (2021b)	High
Vapor pressure	No data identified		
Vapor density	No data identified		
Water solubility	No data identified		
Octanol/water partition coefficient (log K_{OW})	No data identified		
Octanol/air partition coefficient (log K_{OA})	No data identified		
Henry's law constant	No data identified		
Flash point	No data identified		
Autoflammability	No data identified		
Viscosity	No data identified		
Refractive index	1.4054–1.4088 at 20–25 °C	Elsevier (2021b)	High
Dielectric constant	No data identified		

[a] Measured unless otherwise noted
[b] "Data Quality Rating" apply to all references listed in this table

A.1.3 Endpoint Assessments

The physical and chemical property values selected for use in this risk evaluation for D4 degradants are given in Table_Apx A-1, Table_Apx A-2, Table_Apx A-3, and Table_Apx A-4. These values were updated based on systematic review results added since the publication of the *Final Scope of Risk Evaluation for Octamethylcyclotetra- siloxane (D4) – Supplemental File: Data Extraction and Data Evaluation Tables for Physical and Chemical Property Studies for D4 Degradants* (U.S. EPA, 2022a).

A.1.3.1 Physical Form

Only one source was identified and evaluated as a high-quality physical form datum for DMSD. Elsevier (2021c) reported DMSD as a crystal-phase with interplanar spacing and leafs. (Elsevier, 2021d) also reported three high-quality physical form data for dimer diol. Dimer diol is described as a needle-shaped, monoclinic, white crystal. For trimer and tetramer diols, no physical form data was identified.

A.1.3.2 Melting Point

For DMSD, Elsevier (2021c) reported nine high-quality melting point data that ranged from 94.5 to 101 °C. Seven sources reported melting point values from DMSD in a solvent, while two other sources did not report a solvent. The average melting point of those nine data is 98.8 ± 1.56 °C and is selected for use in this risk evaluation.

Elsevier (2021d) reported 19 high-quality melting point data for dimer diol. One melting point datum was reported at 121 °C and the remaining 18 melting point data ranged from 62 to 68 °C. Out of all the melting point data, only eight data reported the solvent used in their studies. The calculated average melting point of those 18 melting point data (excluding the outlier, 121 °C) is 65.5 ± 2.17 °C. Haynes (2014a) reported a melting point of 66 °C, which is in close agreement with the average melting point of Elsevier (2021d).

Elsevier (2021a) reported two high-quality melting point data for trimer diol. A melting point was reported at –1.9 °C and another was reported at –23 °C. The calculated average melting point of both melting point data is –12.5 ± 14.92. The standard deviation is very high, indicating that the value of this parameter is not well-defined. Therefore, a range of –23 to –1.9 °C was selected for use in this risk evaluation.

A high-quality melting point was reported for tetramer diol. Elsevier (2021b) reported a melting point of –5 °C and was selected for use in this risk evaluation.

A.1.3.3 Boiling Point

Systematic review extracted and evaluated five high-quality boiling point data for trimer diol. Elsevier (2021a) reported three boiling point data ranging from 79 to 91 °C at 2–3 torr. Elsevier (2021a) also reported two boiling point values of 106 °C at 6 torr and 72–74 °C at 0.3 torr. All the boiling point data were selected for use in this risk evaluation since they all were not measured under standard atmospheric pressure (*i.e.*, 760 mm Hg ≈ 760 torr).

Systematic review extracted and evaluated two high-quality boiling point data for tetramer diol. Elsevier (2021b) reported 86–88 °C at 0.4 torr and 97–100 °C at 2 torr. Both boiling point data were selected for use in this risk evaluation since they both were not measured under standard atmospheric pressure (*i.e.*, 760 mm Hg ≈ 760 torr).

No boiling point data were identified for DMSD and dimer diol.

A.1.3.4 Density

Systematic review extracted and evaluated two density data for DMSD. RSC (2021) reported a density of 0.97 g/mL, which is equivalent to 0.97 g/cm^3, and was rated as a medium-quality data. Elsevier (2021c) reported a density ranging from 1.095–1.099 g/cm^3 and was rated as a high-quality data. The high-quality density datum from Elsevier (2021c) was selected for use in this risk evaluation.

Systematic review also extracted and evaluated two sources that had density data for dimer diol. Elsevier (2021d) reported three density data. Two of those density data (1.15 and 1.08–1.1) did not report the experimental temperature so they both were excluded for use in this risk evaluation. The density datum of 1.118 g/cm^3 was reported at 16 °C. Haynes (2014a) reported a density value of 1.095 g/cm^3 at 25 °C. The density data from Haynes (2014a) was selected for use in this risk evaluation because the density was measured under standard environmental temperature (*i.e.*, 20–25 °C).

Systematic review identified a high-quality density data for trimer diol. Elsevier (2021a) reported five density values in the range of 0.991 to 1.0127 g/cm^3 at 20–25 °C. The range of 0.991–1.0127 g/cm^3 at 20–25 °C was selected for use in this risk evaluation because all five data had the same rating, and no information was provided to further distinguish them.

Systematic review identified a high-quality density data for tetramer diol. Elsevier (2021b) reported density values of 0.9881 and 0.9886 at 20 °C. They both were selected for use in this risk evaluation because they both had the same rating, and no information was provided to further distinguish both data.

A.1.3.5 Vapor Pressure

Systematic review extracted and evaluated vapor pressure data for DMSD. Dow Corning (2014) reported a vapor pressure of 18.1 Pa, which is equivalent to 0.1358 mm Hg. These data were evaluated to be uninformative. No vapor pressure data were identified for dimer, trimer, and tetramer diols.

A.1.3.6 Vapor Density

No vapor density data were identified for all four degradants.

A.1.3.7 Water Solubility

Systematic review identified four high-quality water solubility data for DMSD. U.S. EPA (2021b) reported 10.8 and 11 M, which is equivalent to 995,000 and 1.01×10^6 mg/L based on DMSD's molecular weight of 92.17 g/mol. NLM (2021b) reported 10.85 M, which is equivalent to 1×10^6 mg/L based on DMSD's molecular weight of 92.17 g/mol. Elsevier (2021c) reported a water solubility value of 2,450 g/L at 25 °C, which is equivalent to 2.45×10^6 mg/L at 25 °C. The water solubility of 2.45×10^6 mg/L at 25 °C from Elsevier (2021c) was selected for use in this risk evaluation because of two reasons. First, U.S. EPA (2021b) and NLM (2021b) did not report an experimental temperature. Secondly, empirical and measured data are preferred over estimated data.

Systematic review identified five high-quality water solubility data for dimer diol. U.S. EPA (2021a) reported 0.661 and 0.662 M, which are equivalent to approximately 110,000 mg/L based on dimer diol's molecular weight of 166.32 g/mol. NLM (2021a) reported 0.66 M, which is equivalent to approximately 110,000 mg/L based on dimer diol's molecular weight of 166.32 g/mol. Elsevier (2021d) reported two water solubility data as "100 g solvent (water) dissolves 11 g substance at 20 °C" and "100 g solvent (water) dissolves 11.5 g substance at 25 °C," which corresponds to 110,000 and 115,000 mg/L, respectively, at 20–25 °C. The water solubility range of 110,000 to 115,000 mg/L at 20–25 °C from Elsevier (2021d) was selected for use in this risk evaluation because of two reasons, same as aforementioned. First, U.S. EPA (2021a) and NLM (2021a) did not report an experimental temperature. Secondly, empirical and measured data are preferred over estimated data.

No water solubility data were identified for trimer and tetramer diols.

A.1.3.8 Octanol/Water Partition Coefficient (log K_{OW})

Systematic review extracted and evaluated four log K_{OW} data for D4 degradants. A medium-quality study, Dow Corning (2014) incorrectly reported a log K_{OW} value of –0.38 from Xu and Kropscott (2012). The correct log K_{OW} value was –0.41. For this reason, Dow Corning (2014) was excluded for use in this risk evaluation. A high-quality log K_{OW} value of –0.41 ± 0.1 at 20.1 °C was reported for DMSD obtained from a laboratory study using a double-syringe apparatus ((Xu and Kropscott, 2012), as cited by (Elsevier, 2021c)). Kurume Laboratory (2021) reported a high-quality log K_{OW} value of <0.3 at 25 °C for DMSD, which was obtained from a laboratory study using OECD TG 117 (OECD, 2022a). The log K_{OW} data from Xu and Kropscott (2012) was selected for use in this risk evaluation because the study provided a precise measurement. Log K_{OW} values of 0.926 ± 0.035, 0.962 ± 0.049, 1.036 ± 0.042, and 1.099 ± 0.025 at 12, 20, 27, and 35 °C, respectively, were reported for dimer diol from a laboratory study using a double-syringe apparatus (Dow Chemical, 2022b). The same study also reported log K_{OW} values of 2.125 ± 0.249, 2.369 ± 0.104, 2.391 ± 0.112, and 2.512 ± 0.165 at 12, 20, 27, and 35 °C, respectively, for trimer diol using the same method. These empirical log K_{OW} data were selected for use in this risk evaluation. In addition, Dow Chemical (2022b) also reported log K_{OW} values of 1.018 ± 0.038 and 2.381 ± 0.017 at 25 °C for the dimer and trimer diols, respectively, which were calculated using linear regression of log K_{OW} values on the reciprocal of absolute temperature (T) in Kelvin. However, these data were not selected for use in this risk evaluation because high-quality empirical log K_{OW} values are available. No log K_{OW} data were identified for tetramer diol.

A.1.3.9 Octanol/Air Partition Coefficient (log K_{OA})

Systematic review extracted and evaluated a high-quality log K_{OA} data for DMSD. Xu and Kropscott (2012) reported a log K_{OA} value of 6.4 ± 0.31 at 20.1 °C. This log K_{OA} datum is selected for use in this risk evaluation. No log K_{OA} data were identified for dimer, trimer, and tetramer diols.

A.1.3.10 Henry's Law Constant

Through systematic review, two high-quality log K_{AW} data for DMSD, and dimer and trimer diols were extracted and evaluated. Xu and Kropscott (2012) reported a log K_{AW} value of –6.84 ± 0.34 at 20.1 °C for DMSD, which is equivalent to 3.48×10^{-9} atm·m^3/mol at 20.1 °C, using Equation 2-1. Dow Chemical (2022b) reported log K_{AW} values of –4.957 ± 0.037, –4.661 ± 0.064, –5.153 ± 0.038, and –4.261 ± 0.095 at 12, 20, 27, and 35 °C, respectively for the dimer diol. These log K_{AW} values are equivalent to 2.58×10^{-7}, 5.25×10^{-7}, 1.73×10^{-7}, and 1.39×10^{-6} atm·m^3/mol at 12, 20, 27, and 35 °C, respectively, using Equation 2-1. For the trimer diol, the log K_{AW} values were –4.320 ± 0.136, –4.291 ± 0.090, –4.107 ± 0.127, and –4.340 ± 0.174 at 12, 20, 27, and 35 °C, respectively. These log K_{AW} values are equivalent to 1.12×10^{-6}, 1.23×10^{-6}, 1.93×10^{-6}, and 1.16×10^{-6} atm·m^3/mol at 12, 20, 27, and 35 °C, respectively, using Equation 2-1. Dow Chemical (2022b) also reported log K_{AW} values of –4.769 ± 0.324 and –4.266 ± 0.270 at 25 °C for dimer and trimer diols, respectively, which were interpolated using the function resulting from a linear regression of log K_{AW} values on the reciprocal of absolute temperature (T) in Kelvin. These log K_{AW} values are equivalent to 4.16×10^{-7} and 1.33×10^{-6} atm·m^3/mol at 25 °C, respectively, using Equation 2-1. No Henry's law constant data were identified for tetramer diol.

A.1.3.11 Flash Point

No flash point data were identified for all four degradants.

A.1.3.12 Autoflammability

No autoflammability data were identified for all four degradants.

A.1.3.13 Viscosity

No viscosity data were identified for all four degradants.

A.1.3.14 Refractive Index

Systematic review identified two high-quality refractive index data for DMSD. Elsevier (2021c) reported a refractive index of 1.444 to 1.448 at 25 °C and 1.452 to 1.456 at 25 °C. A refractive index range of 1.444 to 1.456 at 25 °C from Elsevier (2021c) was selected for use in this risk evaluation because both data had the same rating, and no information was provided to further distinguish them.

Systematic review identified two high-quality refractive index data for dimer diol. Elsevier (2021d) reported a refractive index of 1.457 to 1.461 at 25 °C and 1.462 to 1.466 at 25 °C. A refractive index of 1.457 to 1.466 at 25 °C from Elsevier (2021d) was selected for use in this risk evaluation because both data had the same rating, and no information was provided to further distinguish them.

Systematic review identified six high-quality refractive index data for trimer diol. Elsevier (2021a) reported a refractive index ranging from 1.405 to 1.409 at 20–25 °C. This refractive index range was selected for use in this risk evaluation because all of the data had the same rating, and no information was provided to further distinguish them.

Systematic review identified three high-quality refractive index data for tetramer diol. Elsevier (2021b) reported a refractive index ranging from 1.4054 to 1.4088 at 20–25 °C. This refractive index range was selected for use in this risk evaluation because all of the data had the same rating, and no information was provided to further distinguish them.

A.1.3.15 Dielectric Constant

No dielectric constant data were identified for any of the four degradants.

A.1.4 Strengths, Limitations, Assumptions, and Key Sources of Uncertainty

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 dataset. This duplication should be considered as a potential source of uncertainty in the data analyses. However, data-collection procedures and expert judgment were used to minimize this possibility whenever possible.

A.2 Fate and Transport Assessment

A.2.1 Approach and Methodology

After the final scope (U.S. EPA, 2022b) was published, EPA extracted and evaluated environmental fate and transport properties for DMSD. Table_Apx A-5 provides the selected environmental fate data, and the following sections summarize the findings and provide the rationale for selecting these environmental fate characteristics.

Table_Apx A-5. Environmental Fate Properties of DMSD

Property or Endpoint	Value[a]	Reference(s)	Overall Quality Determination
Direct photodegradation	Degraded via photochemical demethylation in water containing nitrate to yield methylsilanetriol and ultimately to silicic acid	Dow Corning (1980)	Medium
	Degraded via photolytic oxidative demethylation reactions in water containing nitrate or nitrite; silicic acid and carbon dioxide were identified as the final byproducts	Buch et al. (1984)	High
Abiotic degradation in water	98% of DMSD volatilized	Lehmann and Miller (1996)	High
Abiotic degradation in soil	Sand: 7.7%/1 week	Lehmann and Miller (1996)	High
	Sandy clay loam: 3.6%/1 week, 30% after 7 weeks		
Aerobic biodegradation in water	3.5%/30 days based on test substance concentration of 1,000 mg/L	Sabourin et al. (1996)	High
	13–14%/279 days based on test substance concentration of 100 mg/L	Sabourin et al. (1999)	
Aerobic biodegradation in soil	Sandy loam: 9% after 244 days	Sabourin et al. (1996)	High
	Sandy loam: 1.1% after 255 days		
	Sandy: 2.64% after 290 days		
	Clay loam: 1.5% after 290 days		
	Sandy loam: 1.59–1.7%/1 week	Lehmann et al. (1998)	High
	Loam: 0.64–0.74%/1 week		
	Sandy clay loam: 0.42–0.5%/1 week		
	Sand: 0.36–0.42%/1 week		
Organic carbon/water partition coefficient (log K_{OC}) (soil)	0.845	Lehmann and Miller (1996)	High

A.2.1.1 Water

The terminal hydrolysis product of D4, DMSD is expected to persist in the aqueous environment. Because DMSD has a Henry's law constant value of 3.482×10^{-9} at 20.1 °C (Xu and Kropscott, 2012), it is not expected to volatilize from aqueous surfaces. This has been demonstrated in qualitative laboratory studies in which DMSD dissolved in distilled water-filled open scintillation vials demonstrated high recovery (>90%) until the water was completely evaporated (Lehmann and Miller, 1996). With its water solubility of 2.45×10^6 mg/L at 25 °C (Elsevier, 2021c) and a log K_{OW} value of –0.41 at 20.1 °C (Elsevier (2021c) citing Xu and Kropscott (2012), DMSD is not expected to adsorb to particles in the water column. In addition, D4 hydrolysis is not the sole source of DMSD formation in water as other cyclic siloxanes hydrolyze readily to oligomer silanols with DMSD as their terminal hydrolysis product (EC/HC, 2008a, 2008b; Brooke et al., 2009a, 2009b; NICNAS, 2020).

Two studies examining aqueous photolysis of DMSD were identified during systematic review. A medium-quality study, Dow Corning (1980) observed DMSD undergoing photochemical demethylation to yield methylsilanetriol (CASRN 2445-53-6) and ultimately to silicic acid. A high-quality study, Buch (1984) also reported that DMSD was degraded via photolytic oxidative demethylation reactions in water containing nitrate (NO_3) or nitrite (NO^{2-}), and the final products were silicic acid and CO_2.

Biodegradation of DMSD is not expected to be an important process in water. A soil bacterium of the genus *Arthrobacter* mineralized 13 to 14 percent of 100 mg/L of ^{14}C-DMSD in a liquid culture over 279 days (Sabourin et al., 1999) and mineralized 3.5 percent per month of 1,000 mg/L of ^{14}C-DMSD in another study (Sabourin et al., 1996).

A.2.1.2 Soil

Two high-quality biodegradation studies on DMSD were identified during systematic review. Lehmann et al. (1998) studied the importance of microbial degradation in removing DMSD from soil. The biodegradation of DMSD was observed in four different soil types after six months under aerobic conditions with silicic acid and CO_2 as its final products. Sabourin et al. (1996) also reported that DMSD was eventually degraded to CO_2 in four different soil types after approximately 250 days.

Appendix B ADDITIONAL INFORMATION ON D4 BIOACCUMULATION

B.1 Accounting for Fish Lipid Content Variation in Mean Bioconcentration Factor Calculation

Because D4 is a very lipophilic chemical (log K_{OW} = 6.488 L/kg (Kozerski and Shawl, 2007)), bioconcentration and accumulation into tissues is expected to vary with organism lipid content. In order to account for interspecies lipid content variation when determining a central tendency BCF for use in a fish ingestion risk analysis (see *Draft Environmental Media and General Population Exposure for Octamethylcyclotetrasiloxane (D4)* (U.S. EPA, 2025a)), BCF values were lipid-normalized prior to averaging. Briefly, the mean empirical BCFs were lipid-normalized following Equation_Apx B-3. The lipid contents and BCF_L values are presented in Table_Apx B-1.

Equation_Apx B-1

$$BCF_L = \frac{BCF_{ww}}{\varphi_{L,Fish}}$$

Where:

BCF_L = Lipid-normalized bioconcentration factor (L/kg-lipid)
BCF_{ww} = Bioconcentration factor using wet weight organism concentration (L/kg)
$\varphi_{L,Fish}$ = Lipid content of fish (kg-lipid/kg-fish)

Two of the laboratory BCF studies reported lipid content for the fish and tissues used in determining BCF (Fackler et al., 1995; Xue et al., 2020). The remaining two studies did not report lipid content, therefore representative lipid contents from studies presenting comprehensive datasets of the same species were used to normalize these values (Dow Corning, 1992, 1993a). Finally, a generic lipid content of 5 percent (OECD, 2012) was applied to the mean BCF_L to adjust back to a representative BCF_{ww} for use in exposure calculations.

Table_Apx B-1. Summary of Mean BCF Normalization to Account for Interspecies Lipid Content Variation

BCF Study	Fish Species	Mean BCF_{ww} (L/kg)	$\varphi_{L,Fish}$ (%)	$\varphi_{L,Fish}$ SD (%)	$\varphi_{L,Fish}$ Source	Mean BCF_L (L/kg-lipid)
Dow Corning (1992)	Rainbow trout (*Oncorhynchus mykiss*)	8,439	10.4	0.4	Dumas et al. (2007)	81,144
Dow Corning (1993a)	Fathead minnow (*Pimephales promelas*)	8,474	2.22	0.85	Ussery et al. (2024)	381,712
Fackler et al. (1995)	Fathead minnow (*Pimephales promelas*)	12,900	6.4	NR	Fackler et al. (1995)	201,563
Xue et al. (2020)	Common carp (*Cyprinus carpio*)	1,922	4.9[a]	1.1	Xue et al. (2020)	39,145

BCF Study	Fish Species	Mean BCF_{ww} (L/kg)	$\varphi_{L,Fish}$ (%)	$\varphi_{L,Fish}$ SD (%)	$\varphi_{L,Fish}$ Source	Mean BCF_L (L/kg-lipid)
Mean BCF_L across all studies						175,891 L/kg-lipid
BCF_{ww} using generic percent lipid content of 5%, $BCF_{5\%}$						8,795 L/kg

NR = not reported

[a] The BCF presented by Xue et al. (2020) was determined from only filet/muscle tissue. The authors provided percent water content and percent lipid content on a dry weight basis. The lipid content applied here is therefore an average derived from those data, which is also summarized in Table_Apx B-2.

Table_Apx B-2. Summary of Carp Water and Lipid Content from Xue et al. (2020)

Sample ID	Water Content (%)	Lipid Content (% of dw)	Dry Mass Content (%)	Lipid content (% of ww)
F1-1	71	12	29	3.5
F1-2	73	17	27	4.6
F1-3	69	18	31	5.6
F2-1	68	19	32	6.1
F2-2	70	14	30	4.2
F2-3	72	9	28	2.5
F3-1	73	16	27	4.3
F3-2	71	12	29	3.5
F3-3	70	14	30	4.2
F4-1	69	23	31	7.1
F4-2	72	26	28	7.3
F4-3	70	24	30	7.2
F6-1	68	22	32	7.0
F6-2	73	17	27	4.6
F6-3	72	22	28	6.2
F8-1	71	15	29	4.4
F8-2	70	13	30	3.9
F8-3	70	16	30	4.8
F10-1	68	17	32	5.4
F10-2	71	18	29	5.2
F10-3	72	22	28	6.2

Sample ID	Water Content (%)	Lipid Content (% of dw)	Dry Mass Content (%)	Lipid content (% of ww)
F16-1	73	13	27	3.5
F16-2	72	15	28	4.2
F16-3	71	16	29	4.6
F24-1	72	17	28	4.8
F24-2	70	14	30	4.2
F24-3	69	21	31	6.5
F32-1	73	16	27	4.3
F32-2	71	17	29	4.9
F32-3	72	18	28	5.0
F40-1	71	14	29	4.1
F40-2	70	21	30	6.3
F40-3	71	18	29	5.2
F48-1	70	19	30	5.7
F48-2	69	15	31	4.7
F48-3	70	17	30	5.1
F56-1	71	13	29	3.8
F56-2	72	14	28	3.9
F56-3	71	16	29	4.6
F64-1	73	15	27	4.1
F64-2	68	14	32	4.5
F64-3	73	17	27	4.6
Mean	**71**	**17**	**29**	**4.9**
Standard Deviation				**1.1**

B.2 Dissolved Organic Carbon and D4 Bioconcentration

For very hydrophobic chemicals such as D4, adsorption to dissolved organic carbon (DOC) present in the water column and fish bioconcentration through gill/respiratory uptake are competing processes in surface water environments. As such, characterizing the extent to which these processes interact is fundamental to understanding downstream exposures to fish consumers. Cantu et al. (2024) demonstrated this dependency using the ADME-B model described in Gobas et al. (2019). Briefly, wet weight (ww) BCF as determined from bioavailable (*i.e.*, dissolved, not adsorbed) D4 can be described by the following equations:

Equation_Apx B-2

$$BCF = \frac{k_{B1}}{k_{BT}}$$

Where:

k_{BT} = Somatic (body) depuration rate constant (d^{-1})
k_{B1} = Gill uptake rate constant (d^{-1})

The depuration rate constant (k_{BT}) may be determined from the depuration phase of a feeding study (*e.g.*, OECD 305), and k_{B1} is the gill uptake rate (d^{-1}) from freely dissolved/bioavailable D4, determined semi-empirically by:

Equation_Apx B-3

$$k_{B1} = \frac{(k_{B2} \times k_{BW})}{1 + C_{DOC} \times K_{DOC}}$$

Where:

k_{B2} = Respiratory elimination rate constant (d^{-1})
k_{BW} = Fish body-water partition coefficient (L/kg, ww)
C_{DOC} = Concentration of dissolved organic carbon in the water column (kg/L)
K_{DOC} = Dissolved organic carbon/water partitioning coefficient (L/kg)

To illustrate how the BCF of D4 can vary with the DOC content in the water column, EPA used the above-described ADME-B model (Gobas et al., 2019) to predict the BCF of D4 varying C_{DOC} from 1 to 10 mg/L, levels typical of U.S. rivers (Breitmeyer et al., 2019). The input values for the BCF model parameters in Equation_Apx B-1 and B-1. Summary of Mean BCF Normalization to Account for Interspecies Lipid Content Variation

BCF Study	**Fish Species**	**Mean BCF_{ww} (L/kg)**	**$\varphi_{L,Fish}$ (%)**	**$\varphi_{L,Fish}$ SD (%)**	**$\varphi_{L,Fish}$ Source**	**Mean BCF_L (L/kg-lipid)**
Dow Corning (1992)	Rainbow trout (*Oncorhynchus mykiss*)	8,439	10.4	0.4	Dumas et al. (2007)	81,144
Dow Corning (1993a)	Fathead minnow (*Pimephales promelas*)	8,474	2.22	0.85	Ussery et al. (2024)	381,712
Fackler et al. (1995)	Fathead minnow (*Pimephales promelas*)	12,900	6.4	NR	Fackler et al. (1995)	201,563
Xue et al. (2020)	Common carp (*Cyprinus carpio*)	1,922	4.9[a]	1.1	Xue et al. (2020)	39,145
					Mean BCF_L across all studies	175,891 L/kg-lipid

BCF Study	Fish Species	Mean BCF$_{ww}$ (L/kg)	$\varphi_{L,Fish}$ (%)	$\varphi_{L,Fish}$ SD (%)	$\varphi_{L,Fish}$ Source	Mean BCF$_{L}$ (L/kg-lipid)
BCF$_{ww}$ using generic percent lipid content of 5%, BCF$_{5\%}$						8,795 L/kg

NR = not reported

[a] The BCF presented by Xue et al. (2020) was determined from only filet/muscle tissue. The authors provided percent water content and percent lipid content on a dry weight basis. The lipid content applied here is therefore an average derived from those data, which is also summarized in Table_Apx B-2.

Table_Apx B-2. Summary of Carp Water and Lipid Content from Xue et al. (2020)

Sample ID	Water Content (%)	Lipid Content (% of dw)	Dry Mass Content (%)	Lipid content (% of ww)
F1-1	71	12	29	3.5
F1-2	73	17	27	4.6
F1-3	69	18	31	5.6
F2-1	68	19	32	6.1
F2-2	70	14	30	4.2
F2-3	72	9	28	2.5
F3-1	73	16	27	4.3
F3-2	71	12	29	3.5
F3-3	70	14	30	4.2
F4-1	69	23	31	7.1
F4-2	72	26	28	7.3
F4-3	70	24	30	7.2
F6-1	68	22	32	7.0
F6-2	73	17	27	4.6
F6-3	72	22	28	6.2
F8-1	71	15	29	4.4
F8-2	70	13	30	3.9
F8-3	70	16	30	4.8
F10-1	68	17	32	5.4
F10-2	71	18	29	5.2
F10-3	72	22	28	6.2
F16-1	73	13	27	3.5
F16-2	72	15	28	4.2

Sample ID	Water Content (%)	Lipid Content (% of dw)	Dry Mass Content (%)	Lipid content (% of ww)
F16-3	71	16	29	4.6
F24-1	72	17	28	4.8
F24-2	70	14	30	4.2
F24-3	69	21	31	6.5
F32-1	73	16	27	4.3
F32-2	71	17	29	4.9
F32-3	72	18	28	5.0
F40-1	71	14	29	4.1
F40-2	70	21	30	6.3
F40-3	71	18	29	5.2
F48-1	70	19	30	5.7
F48-2	69	15	31	4.7
F48-3	70	17	30	5.1
F56-1	71	13	29	3.8
F56-2	72	14	28	3.9
F56-3	71	16	29	4.6
F64-1	73	15	27	4.1
F64-2	68	14	32	4.5
F64-3	73	17	27	4.6
Mean	**71**	**17**	**29**	**4.9**
Standard Deviation				**1.1**

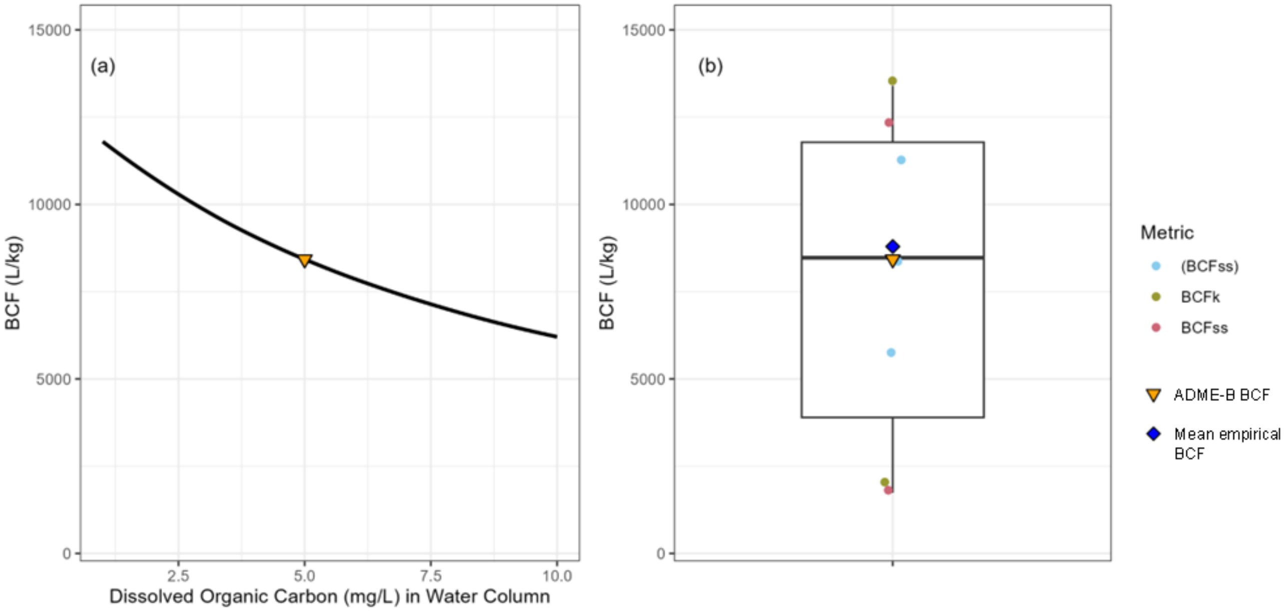
are listed in Table_Apx B-3. A representative DOC concentration of 5 mg/L commonly used in exposure modeling (*e.g.*, default value in the Point Source Calculator (PSC) (U.S. EPA, 2019)) was selected to calculate a BCF of 8,429 L/kg for rainbow trout (*Oncorhynchus mykiss*) based on the D4 elimination kinetics determined by Cantu et al. (2024) (Figure_Apx B-1 (a); BCF at 5 mg-DOC/L indicated by triangle).

Table_Apx B-3. Parameter Values used in ADME-B Model

Parameter	Units	Value	Source
k_{B2}	d^{-1}	0.0004	Cantu et al. (2024)
k_{BW}	d^{-1}	564,777.4	Cantu et al. (2024)
K_{DOC}	L/kg	$10^{5.05}$	Panagopoulos et al. (2015)

Parameter	Units	Value	Source
k_{BT}	d^{-1}	0.0172	Cantu et al. (2024)

Figure_Apx B-1 (b) compares the semi-empirical, ADME-B modeled BCF of rainbow trout at a DOC concentration of 5.0 mg/L against the distribution of reported BCF values identified from empirical studies (*i.e.*, rows (1) to (4) and (8) to (10) of Figure 3-5).



Figure_Apx B-1. D4 BCF Variation with Dissolved Organic Carbon (mg/L) (a) and Central Tendency of Empirical BCF Values (b)

D4 BCF variation in rainbow trout (*Oncorhynchus mykiss*) with dissolved organic carbon (mg/L) in the water column modeled using the ADME-B model (Gobas et al., 2019) described above, triangle indicating BCF at 5 mg-DOC/L of 8,429 L/kg (a); boxplot distribution of reported empirical BCF values compared against the ADME-B BCF value (triangle) and the arithmetic mean of empirical BCF values of 8,795 L/kg (b).

As in Figure 3-5: BCF_{ss} indicates bioconcentration factor determined as a steady-state ratio; BCF_k indicates bioconcentration factor determined by the kinetic rate ratio; (BCF_{ss}) indicates steady-state was assumed but not confirmed.

The semi-empirical ADME-B BCF of 8,429 L/kg agrees well with the central tendency of the empirical values, of which the arithmetic mean is 8,795 L/kg (see Appendix B.2). Because DOC is not traditionally measured during BCF studies, DOC levels from the BCF studies plotted in Figure_Apx B-1 (b) were not reported. Therefore, it cannot be determined how much of the wide variation in reported BCF values for D4 is attributable to differences in DOC. Despite this, it is clear that aqueous DOC concentration can greatly influence the magnitude of D4 BCF and BAF values and is likely a driver of variability in the D4 bioconcentration and bioaccumulation dataset.