ACETIC ACID

This dossier on acetic acid presents the most critical studies pertinent to the risk assessment of acetic acid in its use in hydraulic fracturing fluids and water treatment systems. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Acetic acid is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Acetic acid is a flammable liquid. It readily dissociates in aqueous media to the acetate (H_3C2O_2-) and hydrogen (H+) ions. The acetate ion is readily biodegradable, is not expected to bioaccumulate, and has a low potential to adsorb to soil. Acetic acid is of moderate toxicity to aquatic organisms, in part because of the effect of pH changes from the dissociated hydrogen ion. The acetate ion is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Acetic acid

CAS RN: 64-19-7

Molecular formula: $C_2H_4O_2$

Molecular weight: 60.1 g/mol

Synonyms: Acetic acid, ethanoic acid, ethylic acid, methane carboxylic acid, vinegar acid

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Acetic Acid

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Colourless liquid with a pungent odour.	2	ECHA
Melting Point	16.64°C @ 101.3 kPa	2	ECHA
Boiling Point	117.9°C @ 101.3 kPa	2	ECHA
Density	1040 kg/m^3 @ 25°C	2	ECHA
Vapour Pressure	2079 Pa @ 25°C	2	ECHA

Property	Value	Klimisch score	Reference
Partition Coefficient (log K_{ow})	-0.17 @ 20°C	2	ECHA
Water Solubility	602.9 g/L @ 25°C	2	ECHA
Viscosity	1.056 mPa s @ 25°C	2	ECHA
Dissociation constant (pKa)	4.756 @ 25°C	2	ECHA

Acetic acid readily dissociates in aqueous media to the acetate ($H_3C2O_2^-$) and hydrogen (H^+) ions.

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for acetic acid.

Based on an assessment of environmental hazards, NICNAS identified acetic acid as a chemical of low concern to the environment (DoEE, 2017a). Chemicals of low concern are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

The acetate ion of acetic acid is readily biodegradable, is not expected to bioaccumulate, and has a low potential to adsorb to soil.

B. Partitioning

The pKa of acetic acid is 4.76, indicating that this substance will exist partially in anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts (PubChem).

Volatilization of acetic acid from water and moist soil surfaces is not expected to be an important fate process given a Henry's Law constant of 0.21 Pa-m^3/mole (ECHA). Acetic acid is expected to volatilize from dry soil surfaces based upon its vapour pressure.

Hydrolysis is not expected to be an important environmental fate process since this substance lacks functional groups that hydrolyze under environmental conditions(PubChem).

C. Biodegradation

Acetic acid was readily biodegradable in a non-acclimated freshwater study. Degradation was 96% after 20 days (Price et al., 1974; ECHA) [Kl. score = 2]. Acetic acid is also readily biodegradable under anaerobic conditions (Kameya et al., 1995) [Kl. score = 2].

If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017b).

D. Environmental Distribution

No experimental data are available for acetic acid. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} values from log K_{ow} and the molecular connectivity index (MCI) are 1.153 and 1.0 L/kg, respectively. Based on these values, acetic acid has a low potential for adsorption to soil and sediment and is expected to have very high mobility in soil.

Acetic acid is highly soluble in water and dissociates completely in aqueous solution to acetate and its hydrogen ion. However, the chemistry of the receiving water compartment, such as its pH and the presence of metal ions, may affect the speciation and partitioning of this substance and its buffering capacity (DoEE, 2017c).

E. Bioaccumulation

There are no bioaccumulation studies on acetic acid. Bioaccumulation of acetic acid is not expected to occur because acetic acid dissociates completely in aqueous solution to acetate and its hydrogen ion. Both ions are ubiquitous in the environment. Acetate is naturally found in eukaryotic and prokaryotic cells and is involved in their biochemical pathways.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Acetic acid is of moderate acute toxicity concern to aquatic organisms, in part because of the effect of pH changes from the dissociated hydrogen ion. The acetate ion is of low acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

<u>Acute Studies</u>

Table 3 presents the results of acute aquatic toxicity studies on acetic acid and potassium acetate.

Table 3 Acute Aquatic Toxicity Studies on Acetic Acid and Potassium Acetate

Test Substance	Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Potassium acetate	*Oncorhynchus mykiss*	96-hour LC_{50}	>300.82*	2	ECHA
Potassium acetate	*Danio rerio*	96-hour LC_{50}	>300.82*	2	ECHA
Acetic acid	*Oncorhynchus mykiss*	96-hour LC_{50}	64.8 (measured)	4	ECHA
Acetic acid	*Oncorhynchus mykiss*	96-hour LC_{50}	31.3 – 67.6	4	ECHA
Potassium acetate	*Daphnia magna*	48-hour EC_{50}	>300.82*	2	ECHA
Acetic acid	*Daphnia magna*	48-hour EC_{50}	79.5 (measured)	4	ECHA
Acetic acid	*Daphnia magna*	48-hour EC_{50}	18.9 (measured)	4	ECHA
Acetic acid	*Desmodesmus subspicatus*	72-hour EC_{50}	486.5	4	ECHA

*As the acetate ion.

Chronic Studies

In a 21-day fish (*Oncorhynchus mykiss*) chronic study, the measured NOEC values for 60% and 100% acetic acid were 57.2 and 34.3 mg/L, respectively (ECHA). [Kl. score = 4]

In a 21-day *Daphnia* reproduction study, the measured NOEC for 60% and 100% acetic acid were 80 and 31.4 mg/L, respectively (ECHA). [Kl. score = 4]

In a 21-day *Daphnia* reproduction study, the measured NOEC for 100% acetic acid was 22.7 mg/L (ECHA). [Kl. score = 4]

C. Terrestrial Toxicity

No data are available.

7 CATEGORISATION AND OTHER CHARCTERSTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Acetic acid is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Bioaccumulation of acetic acid is not expected to occur because acetic acid dissociates completely in aqueous media to acetate and its hydrogen ion. Both ions are ubiquitous in the environment.

Acetate is naturally found in eukaryotic and prokaryotic cells and is involved in their biochemical pathways. The log K_{ow} for acetic acid is -0.17. Thus, acetic acid does not meet the screening criteria for bioaccumulation.

The NOECs from the chronic aquatic toxicity studies on acetic acid are >0.1 mg/L. The EC_{50} values for potassium acetate are > 1 mg/L. Thus, acetic acid does not meet the criteria for toxicity.

The overall conclusion is that acetic acid is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for acetic acid.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Acetic Acid	64-19-7	Not a PBT	No	No	No	No	No	No	1	1	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/cm^3	grams per cubic centimetre
g/L	grams per litre
gm/mol	
hPa	hectopascal
IUPAC	International Union of Pure and Applied Chemistry
Kl	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
mPa s	millipascal second
NOEC	no observed effect concentration
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases