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Recommendation for the City of Vernon due to the detection of resorcinol in Kalamalka Lake after the dual-tailer spill accident of 2035

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Table of Contents

Abstract

In this report, the dual-trailer resorcinol spill in Kalamalka Lake was analyzed to determine if the contraction level poses a threat to human and other biological organisms' health. After investigation it was determined that the concentration of resorcinol upon the crash in the hypolimnion is 0.0458mg/kg which does not pose a threat to human oral consumption. This is important because the water from Kalamlak Lake is used at the Mission Hill Drinking Water Treatment Plant, which provides water to the greater Vernon area. In addition, treatments at the DWTP produce the THM chloroform from resorcinol chlorination, but the concentration level is below the MAC for B.C. drinking water standards and is considered safe. During Fall turnover of the lake, the concentration of resorcinol decreases but also allows for air partitioning. However, the concentration of resorcinol in the air is also below the inhalation levels and is considered to not be a threat.

Background

In the summer of 2035 just off Highway 97 a dual-trailer truck carrying 55,000L of resorcinol, swerved, tumbling off the highway down the hill. The trailer crashed into the bottom of Kalamalka Lake and the contents inside dispersed into the lake. Fortunately, the driver made a miraculous leap out of the falling trailer and was not harmed in the incident. However, scientists are concerned about the resorcinol contamination to the lake and decided to do a chemical analysis to determine the risk level of this incidence. Kalamalka Lake is located upstream to the City of Vernon. The lake flows into the Vernon Creek, Okanagan Lake, Okanagan River, Fraser River and eventually into the Pacific Ocean. The main concern is the Mission Hills Drinking Water Treatment Plant that uses its primary source of water from the bottom of Kalamalka Lake and is distributed to the greater Vernon area [4,5]. In this report, investigating the oral in-take limit of resorcinol will be the main concern. Additionally, Kalamalka Lake is a popular tourist attraction with water activities like boating, kayaking and swimming, therefore, precautions for dermal exposure and inhalation will also be covered.

It is important to note this instance as the resorcinol industry continues to grow in Canada and catastrophes like this could become more common. The global resorcinol market from

2024-2030 has grown 6.5% [10], and due to Canada's rapid industrial growth, the chemical resorcinol used in the rubber and tire industry is commonly transported across the country by a dual-trailer (B-train) semitruck. The land area of Canada is made up of about 10% lakes [11], many of which are near highways. Therefore, incidents like trailer spillovers are more likely to occur in the future and this incident report can be used as a preliminary guidance for other incidents in lakes with similar characteristics to Kalamlaka.

Table 1. Characteristics of Kalamalka Lake. [1,2]

Region	Okanagan
Longitude	-119.3538 W
Latitude	50.1589 N
Elevation	392 m
Max depth	144 m
Surface area	25.74 km^2
Secchi depth	11.6 m
Volume of the lake	1.52×10^{12} L [8]
Temperature (summer)	22-27°C
Total organic carbon	3.9 mg/L
Dissolved carbon	4.07 mg/L
Dissolved oxygen	11.81 mg/L
pH	8.24
Turbidity	0.2 NTU

Main Body

Chemical Profile

Structure:

Resorcinol is 1,3-isomer of benzenediol and is the common name for m-Benzenediol, 1,3-Dihydroxybenzene, 3-Hydroxyphenol, m-Hydroxyphenol [12,18]. Its chemical formula is C6H2(OH)2, containing an aromatic ring and two hydroxyl groups one on the second and sixth position. The addition of the two asymmetric hydroxyl groups makes this chemical a polar substance.

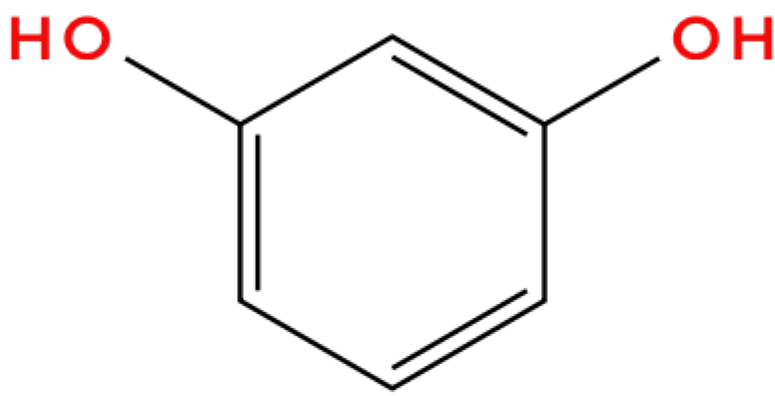


Figure 1. Structure of resorcinol.

Physical and Chemical Properties:

Table 2. Physical and Chemical Properties of Resorcinol.

Molecular Weight [18]	110.11 g/mol
Density [19]	1.3±0.1 g/cm^3
Enthalpy of Evaporation [19]	54 kJ/mol
Solubility [18]	$7.17x10^5$mg/L
Melting Point [21]	108-111°C
Boiling Point [19]	280°C
Vapor Pressure [18]	$4.89x10^{-4}$mm Hg at 25 °C
Henry's Law Constant [21]	$4.96x10^{-9}$
pKa [21]	9.32

Partition Coefficients:

Table 3. Environmental Partition Coefficients of Resorcinol. [19, 21].

Air-Water Partition Coefficient	Kaw	$2.0x10^{-9}$
Octano-Water Partition Coefficient	Kow	7.1
	logKow	0.85 (measured at 25 °C)
Soil Sorption Coefficient	Koc	10.36 (measured)
	logKoc	1.015
Bioaccumulation Factor	BCF	3.2
	logBCF	0.5
	AC/BCF [19]	2.66 at pH 7.4

Use of Resorcinol

Resorcinol is a chemical with a broad set of uses in the manufacturing of hair dyes, pharmaceuticals, flame retardants and fungal creams and is an adhesive in wood coding. However, 50% of the resorcinol industry is for the manufacturing of rubber and tires (21). In tires resorcinol is used to strengthen the rubber-cord interface to reduce rolling and increase stability and durability of tires. These resorcinol enforced tires are used for cars, trucks, fiber-reinforced rubber mechanical goods as well as conveyor belts (21).

Toxicological Effect

Animal Studies:

Studies done on various animals show that resorcinol can cause eye and skin irritation, thyroid issues with acute lethal toxicity levels. It was found that oral exposure was more toxic than dermal exposure, posing a risk to drinking water [21].

Human Effects:

In human cases it has been found that resorcinol is an endocrine disrupting chemical that can cause thyroid and neurological effects if exposed at a very high concentration, typically 50% over the recommended amount in creams and ointments [21]. Topical application of resorcinol in acne and eczema creams have shown some evidence of acute to chronic toxicity after improper use but generally has not shown a serious distribution to the endocrine systems. However, a case study done on an individual who ingested a significant amount of these creams was reported. The symptoms of this patient were unconsciousness, seizures, respiratory failure, leukocytosis and metabolic acidosis which ultimately resulted in death [13].

Chlorination:

Chlorine used at drinking water treatment plants like Mission Hills can cause the halogenation of resorcinol to different DBPs and THMs. The chloration of resorcinol at DWTP produces the THM chloroform in a molar ratio of 1:0.9 resorcinol to chloroform [7]. At low levels chloroform causes dizziness, headaches and at higher levels it results in difficulty breathing, liver and kidney damage [14].

Environmental Entry Characteristics

Table 4. Characteristics of resorcinol and Kalamlaka Lake that affect the entry.

Resorciol		**Kalamalka Lake**	
Solubility [18]	$7.17x10^5$mg/L	foc [16]	0.5%
Density [19]	1.3 g/cm^3	Stratification	Summer
Molar Mass [19]	110.11 g/mol	Mixing	Fall
		Hypolimion [17]	70% (1064x10^12L)

Predicted Concentration

The concentration of resorcinol was first calculated as a liquid solution in the dual-trailer based on its solubility. Once the dual-trailer spilled into the hypolimnion the solution was diluted giving a new concentration. In the hypolimnion resorcinol is exposed to sediments at the bottom of the lake therefore, the Kd must be taken into consideration giving a new concentration after soil sorption (Cw after soil sorption in the hypolimnion). In Fall, turnover occurs and there is no longer a hypolimnion layer, the lake including the resorcinol gets mixed. This allows partitioning into the air resulting in another new concentration of resorcinol in the lake (Cw after turnover and air partitioning).

Table 5. Summary of resorcinol concentrations in Kalamalka Lake.

Type of concentration value	Value (mg/kg bw)
Cw (after soil sorption in the hypolimnion)	0.0458
Cw (after turnover and air partitioning)	0.0319
Ca (air)	$6.41x10^{-11}$

Predicted calculations were made assuming that 100% of the resorcinol solution in the dual-trailer spilled directly into the hypolimnion, and that the hypolimnion accounts for 70% of Kalamlaka Lake [17]. Other assumptions are that the foc for the lake is 0.5% based on the oligotrophic status of the lake [9, 16].

In addition the predicted concentration of chloroform at the DWTP is 0.0382 mg/L, assuming a 1:1 molar ratio from the chlorination of resorcinol to chloroform.

Regulations

Resorcinol:

Table 6. Human exposure limits of resorcinol to the general public and workers in the rubber, tired, and hairdress industry according to the European Chemicals Agency based on a rat study. [22].

Exposure Pathway	Exposure Limit
Oral (general public)	0.4 mg/kg dw (DNEL)
Inhalation (workers)	0.8 mg/kg bw (DNEL)
Dermal (general public)	20 mg/kg dw (DNEL)
Dermal (workers)	40 mg/kg dw (DNEL)

It is important to note the oral, inhalation and dermal exposure limits of resorcinol in regards to the lake contamination due to Kalamlak's high tourist traffic. In the fall during turnover of the lake, dermal and inhalation exposure becomes a concern. Whereas during the summer in the hypolimnion where the crash first happened, oral exposure from drinking water is the main concern.

Chloroform:

The THM chloroform that is produced when resorcinol reacts with chlorine from drinking water treatment plants is also regulated in Canadian drinking water. The MAC for all THMs including chloroform is 100 mg/L [15].

Environmental Distributions

Table 7. Environmental distribution factors of resorcinol. [21].

Koc	10.36
Kow	7.1
Kaw	$2.0x10^{-9}$
Kd	0.00518
BCF	3.2

The Koc and Kow of resorcinol is relatively low meaning that it has high mobility in the soil, with most of it staying in the water column rather than binding to soil particles as well as the low Kd confirms this. The low Kaw also shows that very little resorcinol will partition into the air. The low BCF also indicates that resorcinol does not bioaccumulate or biomagnify in the ecosystem, meaning it will mainly stay in the water. Since the primary location of resorcinol is in the water remediation would need to occur there to eliminate the risk to drinking water.

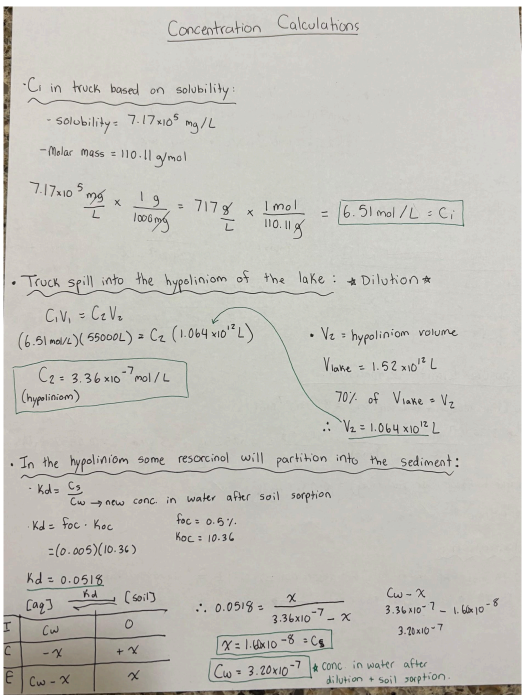
Impact Assessment

The impact of the resorcinol contamination in Kalamalka Lake mainly influences the water quality and people who come in contact with it due to oral or dermal exposure. Due to the relatively low Koc and Kow resorcinol will stay in the water column. In addition the low Kd value also confirms that resorcinol will mainly stay in the water and not bind to soil. Since a majority of the resorcinol partitions into the water, the main concern is the use of Kalamalka Lake as a source of water for the Mission Hills Drinking Water Treatment Facility that provides water to the greater Vernon area. The concentration of resorcinol in the water is $3.20x10^{-7}$ mol/L (0.0485 mg/kg), which is the highest in the summer when the dual-trailer crash leaked into the hypolimnion. The DWTP takes water from the hypolimnion layer as it travels to the facility. Once at the facility the water is chlorinated which has the potential to produce 0.0328 mg/L of chloroform. The exposure limit of chloroform in drinking water is 0.100 mg/L which is greater than the amount in the system. Upon fall turnover, $4.48x10^{-16}$ mg/L ($6.41x10^{-11}$ mg/kg) of resorcinol will partition into the air and allow it to be inhaled. While the remaining $2.23x10^{-7}$(0.0319 mg/kg) stays in the water column.

Conclusion

In conclusion, the concentration of resorcinol in the hypolimon of the lake, and after turnover do not pose a threat to human or biological organisms' health. In addition, the concentration of resorcinol in the air after turnover is minimal and safe as well as the formation of chloroform in the Mission Hill drinking water treatment plant. Therefore, it is safe to assume no removal strategies or hazard alerts to the public need to be made. In another event like this, similar actions could be made.

Appendix



Concentration Calculations

- C_i in truck based on solubility:
  - solubility = 7.17×10^5 mg/L
  - Molar mass = 110.11 g/mol

$7.17 \times 10^5 \frac{mg}{L} \times \frac{1\ g}{1000\ mg} = 717 \frac{g}{L} \times \frac{1\ mol}{110.11\ g} = 6.51\ mol/L = C_i$

- Truck spill into the hypoliniom of the lake: ★ Dilution ★

$C_1V_1 = C_2V_2$

$(6.51\ mol/L)(55000L) = C_2(1.064 \times 10^{12} L)$

$C_2 = 3.36 \times 10^{-7}$ mol/L (hypoliniom)

- V_2 = hypoliniom volume

$V_{lake} = 1.52 \times 10^{12}$ L

70% of $V_{lake} = V_2$

$\therefore V_2 = 1.064 \times 10^{12}$ L

- In the hypoliniom some resorcinol will partition into the sediment:
  - $Kd = \frac{C_s}{C_w}$ → new conc. in water after soil sorption
  - $Kd = foc \cdot Koc$ = (0.005)(10.36)

foc = 0.5%

Koc = 10.36

Kd = 0.0518

[aq] ⇌ (Kd) [soil]

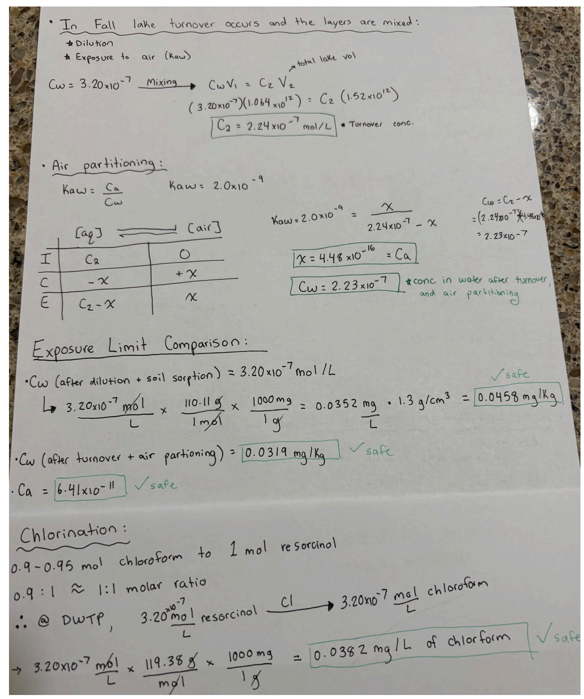
	[aq]	[soil]
I	Cw	0
C	−x	+x
E	Cw − x	x

$\therefore 0.0518 = \frac{x}{3.36 \times 10^{-7} - x}$

$x = 1.60 \times 10^{-8} = C_s$

$C_w - x$: $3.36 \times 10^{-7} - 1.60 \times 10^{-8}$ = 3.20×10^{-7}

$C_w = 3.20 \times 10^{-7}$ ★ conc in water after dilution + soil sorption.



- In Fall lake turnover occurs and the layers are mixed:
  - ★ Dilution
  - ★ Exposure to air (Kaw)

$C_w = 3.20 \times 10^{-7}$ —Mixing→ $C_wV_1 = C_2V_2$ (total lake vol)

$(3.20 \times 10^{-7})(1.064 \times 10^{12}) = C_2(1.52 \times 10^{12})$

$C_2 = 2.24 \times 10^{-7}$ mol/L ★ Turnover conc.

- Air partitioning:

$Kaw = \frac{C_a}{C_w}$ $Kaw = 2.0 \times 10^{-9}$

[aq] ⇌ [air]

	[aq]	[air]
I	C_2	0
C	−x	+x
E	$C_2 - x$	x

$Kaw = 2.0 \times 10^{-9} = \frac{x}{2.24 \times 10^{-7} - x}$

$x = 4.48 \times 10^{-16} = C_a$

$C_w = C_2 - x = (2.24 \times 10^{-7}) - (4.48 \times 10^{-16}) = 2.23 \times 10^{-7}$

$C_w = 2.23 \times 10^{-7}$ ★ conc. in water after turnover, and air partitioning

Exposure Limit Comparison:

- Cw (after dilution + soil sorption) = 3.20×10^{-7} mol/L

→ $3.20 \times 10^{-7} \frac{mol}{L} \times \frac{110.11\ g}{1\ mol} \times \frac{1000\ mg}{1\ g} = 0.0352 \frac{mg}{L} \cdot 1.3\ g/cm^3 = 0.0458$ mg/Kg ✓ safe

- Cw (after turnover + air partioning) = 0.0319 mg/Kg ✓ safe
- Ca = 6.41×10^{-11} ✓ safe

Chlorination:

0.9 − 0.95 mol chloroform to 1 mol resorcinol

0.9 : 1 ≈ 1:1 molar ratio

$\therefore$ @ DWTP, $3.20 \times 10^{-7} \frac{mol}{L}$ resorcinol —Cl→ $3.20 \times 10^{-7} \frac{mol}{L}$ chloroform

→ $3.20 \times 10^{-7} \frac{mol}{L} \times \frac{119.38\ g}{mol} \times \frac{1000\ mg}{1\ g} = 0.0382$ mg/L of chlorform ✓ safe

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