Comparing inhalation and ingestion exposure to chemical contaminants and odorants in mixtures

D. L. Gallagher, K. Phetxumphou and A. M. Dietrich

ABSTRACT

Chemical spills polluting drinking water are often mixtures with each chemical having unique characteristics for partitioning, toxicity, and odour leading to significant differences in human risk exposures. A 2014 chemical spill of crude (4-methylcyclohexyl)methanol (MCHM) resulted in a $126 million USD fine to the water utility. The spill consisted of at least ten chemicals including 34% *cis*- and 60% *trans*-4-MCHM and 0.7% *cis*- and 0.3% *trans*-methyl-4-methylcyclohexanecarboxylate (MMCHC). While a very minor component, *trans*-MMCHC contributed substantially to odour because of its high Henry's Law Constant, 2.23×10^{-2} at 40 °C showering, and low odour threshold concentration (OTC), 0.02 ppb-v, air. Using USEPA risk assessment parameters in a 15-minute shower model with influent concentration of 42 ppb-aq *cis*- and *trans*-4-MMCHC, representative of initial spill concentrations in the distribution system, adult ingestion and inhalation for *trans*-MMCHC were almost equal, 4.00×10^{-4} and 4.26×10^{-4} mg/kg/d, respectively. For children, inhalation doses exceeded ingestion dose: 1.72×10^{-3} mg/kg/d versus 0.93×10^{-3} mg/kg/day *trans*-MMCHC. This exposure assessment with varying OTC for crude MCHM chemicals reinforces considering chemical, physical, and biological properties of all chemicals in the spill. Consumers aware of their exposure to chemicals in drinking water lost consumer confidence; the water utility was required to compensate individuals and businesses for financial losses.

Key words | chemical spill, exposure, ingestion, inhalation, odour, mixture

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INTRODUCTION

The rupture of a poorly maintained chemical storage tank owned by Freedom Industries allowed nearly 38,000 L of licorice-smelling crude (4-methylcyclohexyl)methanol (MCHM) to enter the Elk River, which was the drinking water supply for over 300,000 people in Charleston, West Virginia and surrounding counties. Contaminated Elk River water was processed through a conventional drinking water plant. Attempts to treat and remove the chemical contaminants with addition of activated carbon and potassium permanganate were ineffective (Weidhaas *et al.* 2017). Licorice-smelling drinking water was distributed to consumers who noticed the odorous drinking water early in the morning of January 9, 2014. By 6 PM that evening, a 'do-not-use the water order' was issued by government officials. Consumers were told not to drink, wash, or use water; the 'do-not-use the water order' remained in place for up to a week and a half for some sections of the distribution system (Gallagher *et al.* 2015; Schade *et al.* 2015). Communication through public notification and social media was effective. In a post-spill survey, 89% of affected consumers reported knowing about the spill the day that it occurred (Savoia *et al.* 2015).

Minimizing exposure was critical as there was little technical and/or toxicological data for crude MCHM, which is an unregulated industrial chemical consisting of a mixture of predominantly ten substituted cyclohexanes (Figure 1)

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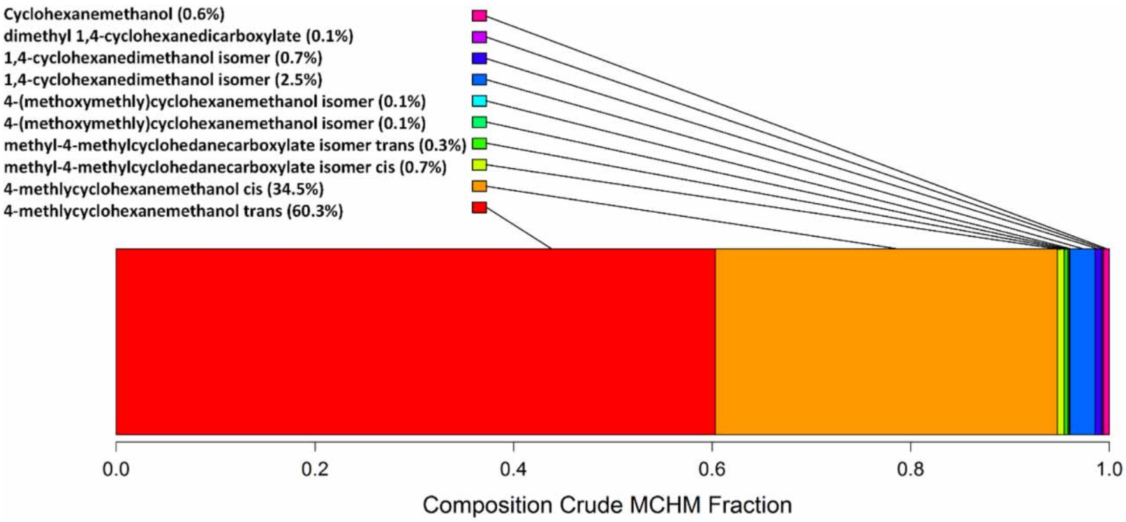

Figure 1 | Chemical composition of crude MCHM that spilled into the Elk River and contaminated drinking water in West Virginia (Eastman Chemical Company 2011; Gallagher *et al.* 2015).

(Gallagher *et al.* 2015). Even though at the time of the spill it was known that crude MCHM was a mixture of chemicals, the liquid–liquid extraction gas chromatography/mass spectrometry (GC/MS) monitoring method used at the water company only measured and reported the two major isomers of crude MCHM (*cis*- and *trans*-4-MCHM) as total 4-MCHM rather than the individual species. Monitoring during and for months after the spill by the United States Geological Survey, which used a purge-and-trap-GC-MS method, demonstrated that both the 4-MCHM isomers and minor components, methyl-4-methylcyclohexanecarboxylate (MMCHC) isomers, had high volatility, occurred in tap water, and could cause odours (Foreman *et al.* 2015).

Estimated Odour Threshold Concentration (OTC) and Odour Recognition Concentration (ORC) were developed as biomarkers of human exposure of crude MCHM although the analytical chemical reporting limit was showing non-detects at less than 10 μg/L-aq at that time. A consumer odour panel of 60 participants reported the crude MCHM OTC and ORC as 0.55 μg/L-aq and 7.44 μg/L-aq, respectively, in early March 2014 (McGuire *et al.* 2014). These findings supported consumer odour observations in Charleston.

Immediately and for days after the spill, many people reported illnesses, such as gastrointestinal symptoms (nausea, vomiting, diarrhea, and/or abdominal cramps) skin irritation (rashes and itching), central nervous system symptoms (headache and dizziness) and respiratory symptoms; many of those affected sought medical help (WVBPH & ATSDR 2014; Schade *et al.* 2015; Thomasson *et al.* 2017). It required about a week for the US Centers for Disease Control and Prevention (US CDC) to issue an ingestion health advisory of 1 mg/L-aqueous for the crude MCHM mixture (US CDC 2014). Even though exposure through smelling the chemicals was a main complaint of consumers, respiratory illness was one of the three main reasons people sought medical help (Thomasson *et al.* 2017). An inhalation advisory of 0.01 ppm-v of inhalable air would not be issued until approximately 6 months after the spill (US EPA 2014). While a consumer survey indicated that 69% of the affected population complied with instructions to not drink the tap water, few consumers reported complying with other behaviour modifications like not using contaminated water for washing (Savoia *et al.* 2015). In another survey, 37% of affected consumers reported continual use of tap water for any household purpose during the time of the spill, with showering being the most common use (Burrer *et al.* 2017). Thus, many consumers subjected themselves to inhalation exposure. For months after the 'do-not-use the water order' was lifted, consumers were reluctant to use the tap water. Approximately three months after the spill, only 34% of consumers reported using the tap water for drinking, and only 36% believed the water was safe (Burrer *et al.* 2017).

A maximum reported concentration of 3,800 μg/L-aq combined *cis*- and *trans*-4-MCHM (total 4-MCHM) was measured in the distribution system during the early days of the spill. Recent data from court records suggest that aqueous concentrations in drinking water during the early hours of the spill may have been in the range 13,000–100,000 μg/L-aq (Ward 2016c). Days and weeks later, limited monitoring data demonstrated that water concentrations subsequently fell below the US CDC health advisory of 1 mg/L in water for combined *cis*- and *trans*-4-MCHM. Even so, consumers living in the affected area were occasionally plagued by licorice-odours when using drinking water in residential homes, schools, and local buildings. Odours were especially noticeable when warm and hot water were used (Sain *et al.* 2015; Schade *et al.* 2015). Eventually, the saturated carbon filters at the water treatment plant were confirmed as one source of continued contamination and lingering odour; replacement of the carbon began about 3 months after the initial spill (Constantino 2014). Subsequent research confirmed that activated carbon could both remove and release odorous MCHM (Ahart *et al.* 2016). The US EPA short-term air-screening level of 0.01 ppm-v for inhalable air (US EPA 2014) issued in July 2014 was more than a factor of 150 higher than the odour threshold for individual components of the crude MCHM mixture (Gallagher *et al.* 2015; Sain *et al.* 2015). While residents of Charleston, West Virginia repeatedly complained of odours even when not drinking the water, inhalation exposure was not investigated by water utility personnel or governmental agencies during or after the spill.

A year after the spill, residents of West Virginia were still reluctant to drink water distributed by the water treatment plant and not all their questions and concerns had been answered (Ward 2015). The legal ramifications of the spill took longer than two years to settle and are summarized below.

- Freedom Industries (owner of ruptured crude MCHM tank): This company declared bankruptcy soon after the spill. In February 2016, a US Federal Court fined the company a $900,000 USD 'symbolic' fine because a bankrupt company would not pay (Ward 2016a). The company's president, Gary Southern, received a one-month jail sentence and $20,000 USD fine as did the former co-owner, Dennis Farrell (Ward 2016a, 2016b). Four other employees were charged with violations of the Clean Water Act, the Refuse Act, and permitting violations (Ward 2016a).
- Eastman Chemical Company (manufacturer of crude MCHM): Eastman Chemical will be required to pay $25 million USD because they failed to properly caution Freedom Industries about the potential dangers of MCHM and did not take appropriate actions when information pertaining to the poor state of the chemical storage tanks was made known (Ward 2016b).
- West Virginia American Water (the water utility): In the class action settlement of Crystal Good vs. American Water, West Virginia American Water will have to provide $126 million USD to compensate over 224,000 residents, 7,300 businesses, and an undetermined figure of hourly wage workers (Ward 2016b). The lawsuits found that American Water failed to store treated water that would have allowed for temporary closing of the water intake. The water utility also failed to properly maintain or even destroyed water samples taken early after the spill (Ward 2016c). Additionally, the water utility did not have a suitable plan in place to respond to such chemical spills (Ward 2016c). Within the settlement, American Water will not be able to increase water rates to cover the cost of the settlement; the money should come from investors, stockholders, and insurance policies (Ward 2016b).

A 2017 American Water Works Association survey found that the water industry's most important regulatory concern is chemical spills (AWWA 2017). While chemical spills occur worldwide and disrupt drinking water supplies, distribution systems, and consumers' lives and livelihoods (Zhang *et al.* 2011; Jiang *et al.* 2012), this chemical spill and drinking water contamination in West Virginia highlights many important issues related to drinking water protection, consumer protection, and consumer satisfaction (Weidhaas *et al.* 2016), including:

1. lack of source water protection policies;
2. lack of monitoring methods for industrial chemicals in water;
3. lack of detailed exposure assessment for both inhalation and ingestion;

4. lack of human toxicity data;
5. lack of attention to consumer communication and perception.

While all of these issues need to be addressed to provide safe and sustainable drinking water, the focus of this document is on Item 3: *lack of detailed exposure assessment for both inhalation and ingestion*. The aim is to compare inhalation and ingestion exposure for adults and children under conditions that occurred during the crude MCHM spill.

METHODS

The biological and physicochemical data used to develop a comparison of human inhalation during showering versus ingestion exposure are summarized in Tables 1 and 2. Inhalation and ingestion doses were estimated by calculation of a daily dose (mg/kg/d) based on US EPA risk assessment parameters (US EPA 2014). Risk parameters included adults weighing 70 kg, ingesting 2 L/d of water, and inhaling 20 m^3/d of air. For children, risk parameters were weighing 10 kg, ingesting 1 L/d of water, and inhaling 17.3 m^3/d of air. The weight and breathing rate for the child are very conservative values selected by US EPA to establish a low air exposure concentration for the screening level of MCHM (US EPA 2014). A previously published shower model, as described by Sain *et al.* (2015), was applied to assess exposure to chemicals with a concentration of 4,000 ppb-aq combined *cis*- and *trans*-4-MCHM, which represents a high concentration detected in the distribution system during the spill. Since the MMCHC isomers represent about 1% of the concentration of the 4-MCHM isomers, 42 μg/L-aq combined *cis*- (28 μg/L-aq) and *trans*-4-MMCHC (14 μg/L-aq) was used as the influent MMCHC concentration in the shower model. Inhalation doses were calculated by integrating the area under the predicted shower concentration curves versus time data. Odour activity values (OAV) represent the ratio of a chemical's concentration in a mixture to its OTC (Grosch 1994). Statistical analyses and modelling were performed in R (R Core Team 2015).

Table 1 | Descriptors and odour threshold concentrations (OTC) for major odorous chemicals in crude MCHM

Compound	Dominant odour descriptors	OTC ppb-v, air
cis-4-MCHM	Fermented fruit[a]	120[a]
trans-4-MCHM	Licorice[a]	0.06[a]
cis-MMCHC	Sweet, Fruity[b]	1.828[b]
trans-MMCHC	Sweet, Fruity[b]	0.021[b]

[a]Gallagher *et al.* (2015).
[b]Phetxumphou *et al.* (2016).

RESULTS AND DISCUSSION

Establishing which chemicals resulted in higher human exposure for both ingestion and inhalation is challenging because the fate, transport, and odour properties of specific chemical compounds in crude MCHM varied, as shown in Tables 1 and 2. For odorous chemicals in drinking water, the human sense of smell confirms exposure even when

Table 2 | Physical and chemical properties for *cis*- and *trans*-4-MCHM and for *cis*- and *trans*-MMCHC

		Dimensionless, air/water Henry's Law Constant			Diffusivity m^2/s	
Compound	Aqueous solubility mg/L	22 °C	40 °C	ΔH Aqueous vapor (J/mol)	Liquid	Gas
cis-4-MCHM	1,300[a]	2.00×10^{-4} [b]	6.38×10^{-4} [b]	40,600[b]	7.36×10^{-10} [c]	6.71×10^{-6} [c]
trans-4-MCHM	1,010[a]	4.85×10^{-4} [b]	1.52×10^{-3} [b]	27,200[b]		
cis-MMCHC	173[c]	1.00×10^{-2} [d]	1.50×10^{-2} [d]	17,313[d]	6.84×10^{-10} [c]	6.37×10^{-6} [c]
trans-MMCHC	173[c]	1.38×10^{-2} [d]	2.23×10^{-2} [d]	20,599[d]		

[a]Dietrich *et al.* (2015).
[b]Sain *et al.* (2015).
[c]US EPA (2012).
[d]Phetxumphou *et al.* (2016).

quantitative chemical monitoring data are lacking (Dietrich & Burlingame 2015).

The interaction of the physical–chemical properties (Henry's Law Constant) and biological properties (odour thresholds) results in the media concentrations shown in Figure 2. Influent aqueous concentrations were 4,000 μg/L-aq combined *cis*- and *trans*-4-MCHM with 1% or 42 μg/L-aq combined *cis*- and *trans*-MMCHC. The 4-MCHM isomers dominate with concentrations of 2,545 and 1,455 μg/L-aq for the *trans*- and *cis*- isomers, respectively. MMCHC isomers' concentrations are approximately two orders of magnitude lower, with *trans*-MMCHC having the lowest concentration.

MMCHC isomers have more than an order of magnitude higher Henry's Law Constant than the 4-MCHM isomers, which results in a relative increase in shower air concentrations. MMCHC isomers are also more odorous than their 4-MCHM counterparts, resulting in even greater human detection as measured by OAV. The *trans*- isomers are much more odorous than the *cis*- isomers. *Trans*-MMCHC is three times more odorous (i.e., three times lower OTC) than *trans*-4-MCHM. *Trans*-MMCHC is only 0.3% of the aqueous mass, but leads to approximately 20% of the odour due to its higher volatility and lower OTC.

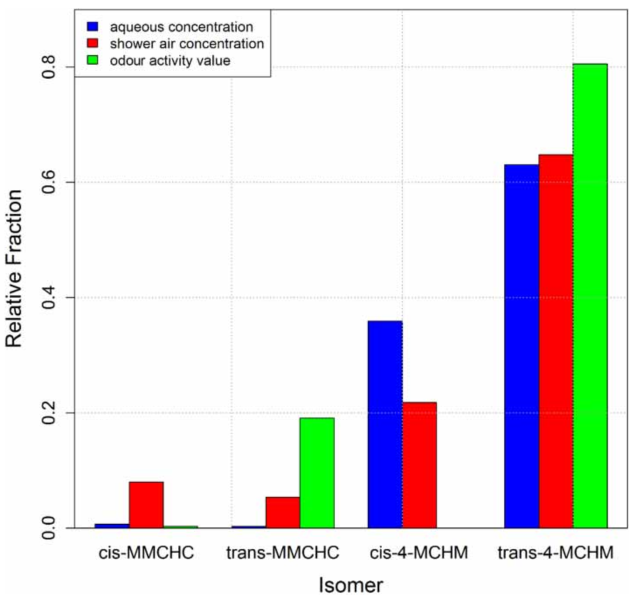

Figure 2 | Changing distributions of components of crude MCHM in water (based on relative μg/L-aq), in shower air after 15 minutes of showering at 40 °C (based on relative ppb-v), and in OAV for human perception during showering.

The odour percentage for *trans*-MMCHC increases slightly as shower time increases, reaching approximately 15% after 2 minutes and 19% after 15 minutes with a concomitant decrease in the *trans*-4-MCHM percentages.

Figure 3 shows the comparison of inhalation versus ingestion doses for adults (Figure 3(a)) and children over time during showering (Figure 3(b)). The high volatility of MMCHC isomers leads to relatively high inhalation doses. At approximately 15 minutes, *trans*-MMCHC doses for adult ingestion and inhalation are approximately equal. After a 10–12 minute shower, children's inhalation exposures exceed their ingestion doses for both isomers.

A comparison of the inhalation and ingestion exposures for individual isomers appears in Table 3. Because of their much higher aqueous concentrations and moderate volatilities, the 4-MCHM isomers have corresponding higher doses for both exposure pathways compared to the MMCHC isomers. In general, approximately 90% of the dose for the 4-MCHM isomers was from ingestion. Although the MMCHC isomers had lower aqueous concentrations, their higher volatilities potentially allowed inhalation exposure to be a more significant route than ingestion. This was always true for children – children had higher exposures to MMCHC isomers through showering than through drinking water. While this research focuses on exposure to individual chemicals in the spill, it is important to acknowledge that consumers are simultaneously exposed to all chemicals, as shown with the total dose entry in Table 3.

Figure 4 shows the development of OAV over time for the two MMCHC isomers during showering. For most people, the odour from the *trans*-MMCHC isomer is readily apparent within seconds and dominates throughout the shower. While the dose for the *cis*-MMCHC isomer was always higher because of its higher aqueous concentration and near equal volatility, the *trans*-MMCHC isomer completely dominates the odour because of its almost 100× lower OTC.

This research confirms that both inhalation and ingestion are substantial routes of exposure to aqueous contaminants. In-depth research on mixtures of trihalomethanes, which included monitoring exposure and human blood and breath concentrations, demonstrated that water-use activities such as showering, bathing, and washing clothes or dishes result in human inhalation

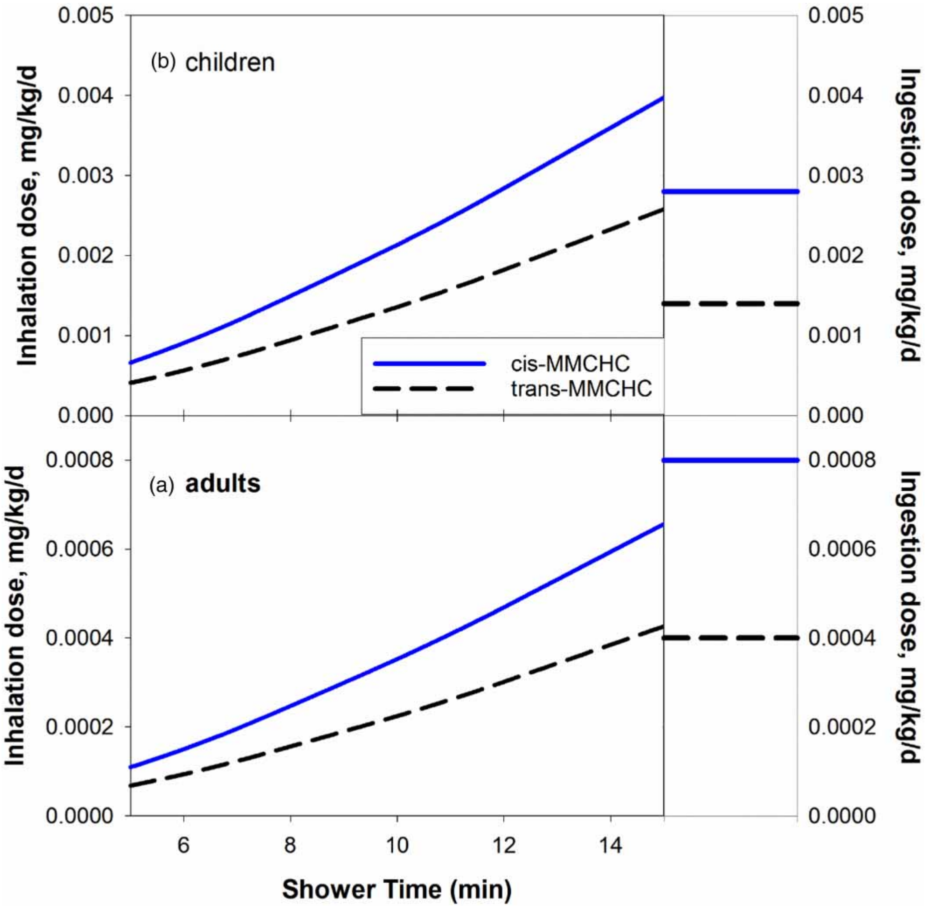

Figure 3 | Inhalation during showering versus ingestion doses for the MMCHC isomers: (a) adult doses; (b) child doses.

exposure to drinking water contaminants (Gordon *et al.* 2006). Inhalation is a more important route of exposure for the two more volatile trihalomethanes, trichloromethane and bromodichloromethane (Gordon *et al.* 2006).

In the study of the chemical mixture, crude MCHM, odour detection was a biomarker for human exposure (McGuire *et al.* 2014; Gallagher *et al.* 2015; Phetxumphou *et al.* 2016). Odour, as an indicator of human exposure, is

Table 3 | Doses of crude MCHM contaminants from showering (15 minute shower at 40 °C) and drinking for adults and children for aqueous concentrations of 2,545 and 1,455 μg/L-aq *trans*-4-MCHM and *cis*-4-MCHM respectively, and 14 and 28 μg/L-aq *trans*-MMCHC and *cis*-MMCHC respectively

	Adult			Child		
Contaminant	Inhalation in shower (mg/kg/d)	Ingestion of drinking water (mg/kg/d)	Ratio[a]	Inhalation in shower (mg/kg/d)	Ingestion of drinking water (mg/kg/d)	Ratio[a]
trans-MMCHC	0.43×10^{-3}	0.40×10^{-3}	1.07	2.58×10^{-3}	1.40×10^{-3}	1.84
cis-MMCHC	0.66×10^{-3}	0.80×10^{-3}	0.82	3.97×10^{-3}	2.80×10^{-3}	1.42
trans-4-MCHM	4.82×10^{-3}	72.7×10^{-3}	0.07	29.2×10^{-3}	255×10^{-3}	0.11
cis-4-MCHM	1.63×10^{-3}	41.6×10^{-3}	0.04	9.85×10^{-3}	146×10^{-3}	0.07
Total dose, 4 isomers	7.53×10^{-3}	115×10^{-3}	–	45.6×10^{-3}	404×10^{-3}	–

[a]Inhalation dose divided by ingestion dose.

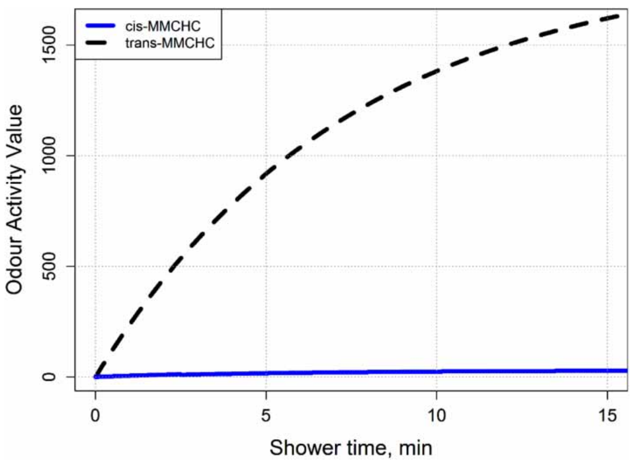

Figure 4 | OAV during showering time for the MMCHC isomers.

readily implemented and reported without expensive and potentially invasive monitoring of human body fluids. While not all chemicals are odorous, many are. Depending on the concentration present in the water and the chemical's OTC, it may be readily detected by the sense of smell. If consumers are smelling chemicals in their water, then they are exposed. The drinking water industry recently ranked chemical spills as its most important current regulatory concern, followed by point source pollution (AWWA 2017). Attention focused on inhalation exposure and interpreting consumer complaints related to taste and odour can be an asset for identifying and controlling drinking water contamination as well as maintaining and improving consumer confidence. Not heeding consumer responses to contamination, as was done in the crude MCHM contamination of the Elk River and West Virginia American Water Company, resulted in loss of consumer confidence (Burrer *et al.* 2017) in the drinking water and costly legal settlements (Ward 2016b, 2016c) for the water utility.

CONCLUSIONS

Preventing chemical spills through adequate source water protection should be a water industry priority. When spills occur, utilities need to be prepared for such events to limit drinking water contamination and public health concerns. To protect individual and the public health, there is a vital need to know essential fate and transport properties (such as solubility, Henry's Law Constants, enthalpy), biological properties (toxicity and odour), and exposure routes for each chemical in the spill. For different chemicals, these properties vary by orders of magnitude and affect human exposure risks, even among isomers. Chemicals that are considered minor components because of their percent composition should always be investigated as they can have major human impacts. Additionally, air samples are as vital as water samples and should be collected and examined. The ramifications for not protecting the public from inhalable and ingestible waterborne contaminants can result in loss of consumer confidence and costly litigation.

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