Intricacies of odour response to chemicals in mixtures

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Abstract

Chemical spills that contaminate drinking water are often mixtures of chemicals. Each component in a mixture has unique characteristics such as concentration, volatility, aqueous solubility, octanol-water coefficients, toxicity, and odour properties that can result in significant differences to human risk exposures. Of the ten cyclohexanes in the 2014 crude (4-methylcyclohexyl)methanol (4-MCHM) spill that contaminated drinking water in Charleston, WV, USA, ^{1}H nuclear magnetic resonance and chromatography determined that the mixture was comprised of 34% *cis*- and 60% *trans*-4-MCHM isomers and 0.7% *cis*- and 0.3% *trans*-methyl-4-methylcyclohexanecarboxylate (MMCHC) isomers. While very minor components, MMCHC isomers were large contributing factors to odours associated with the spill. At typical 40°C showering temperature, Henry's Law Constants were experimentally determined to be 1.50×10^{-2} and 2.23×10^{-2} for *cis*- and *trans*-MMCHC, respectively, which is 20-50 fold higher than for 4-MCHM isomers. Odour thresholds concentrations (OTCs) were 1.83 and 0.02 ppb-v, air for *cis*- and *trans*-MMCHC, respectively, with both described as predominantly sweet. The OTCs for *cis*- and *trans*-4-MCHM, respectively, were 120 and 0.06 ppb-v, air; the *trans*-isomer had a dominant licorice odour. Application of the shower model revealed that t*rans*-4-MCHM contributed about 82% of odour, but because of *trans*-MMCHC's higher volatility and lower OTC, it contributed to 18% of the odour. This study of human sensory and varying OTC responses to exposure of the crude MCHM spill reaffirms the need to assess chemical, physical, and biological properties of all components within the mixture of chemicals spilled.