February 1986
(edited August 1988)

Toluene, Ethylbenzene and the Xylenes

Guidelines

The aesthetic objectives (AO) for toluene, ethylbenzene and the xylenes in drinking water are:

	AO	
	mg/L	**μg/L**
toluene	*≤ 0.024*	*≤ 24*
ethylbenzene	*≤ 0.0024*	*≤ 2.4*
xylenes (total)	*≤ 0.3*	*≤ 300*

Identity, Use and Sources in the Environment

Toluene, ethylbenzene and the xylenes all belong to a group of organic compounds known as alkyl benzenes. They are single-ring aromatic hydrocarbons with various alkyl groups attached to the ring. Toluene and ethylbenzene contain a methyl group and an ethyl group, respectively, whereas the xylenes contain two methyl groups.

There are three possible xylene isomers: 1,2-, 1,3- and 1,4-dimethylbenzene; these will be referred to as the o- (ortho), m- (meta) and p- (para) xylene isomers, respectively, for the remainder of this review. The xylenes are for the most part manufactured and marketed as a mixture of the isomers, and this mixture will be termed xylene in this report.

Toluene, molecular formula C_7H_8, is a clear, colourless liquid at room temperature, and it has a sweet, pungent, benzene-like odour.[1] It has a boiling point of 110.6°C[2,3] and a vapour pressure of 3.8 kPa at 25°C, and its density is 0.8869 g/mL at 20°C. Toluene is slightly soluble in fresh water (535 mg/L) at 25°C.[4] Its log octanol–water partition coefficient (K_{ow}) is about 2.74.[5]

Ethylbenzene, molecular formula C_8H_{10}, is a flammable, colourless liquid with an aromatic odour. It has a boiling point of 136.25°C,[2,3] and at 25°C its density is 0.866 g/mL.[6] In distilled water at 25°C, ethylbenzene has a solubility of 161.2 mg/L.[7] Ethylbenzene has a K_{ow} of 3.15.[5]

The molecular formula of the three xylene isomers is C_8H_{10}, and all ar e colourless liquids at room temperature. Pure p-xylene forms colourless plates or prisms at 13°C, whereas the other two isomers are liquids.[8] The boiling points for the xylenes range from 137 to 144°C,[2,3] and K_{ow}'s are 2.77, 3.20 and 3.15 for the o-, m- and p-isomers, respectively.[5]

The primary source of these alkyl benzenes in the environment is the petroleum industry and, to a lesser extent, the coke industry. Toluene, ethylbenzene and the xylenes are all used extensively as solvents and as raw materials in the synthesis of a variety of chemicals. All are used to some extent in the rubber and plastics industries, and all have been used as gasoline additives.

Seventy percent of all toluene produced is used in the manufacture of benzene.[1] Toluene is also commonly used as a solvent or thinner in paints, lacquers and adhesives and as a precursor of other widely used chemicals, such as toluene diisocyanate, phenol, nitrotoluenes and vinyl toluenes.

Ethylbenzene is primarily used in the manufacture of styrene. In 1975, 98% of all ethylbenzene produced in the United States was used as the raw material for styrene manufacture.[9] Ethylbenzene is also present in xylene (up to 20%), and this mixture is used as a diluent in the paint industry, in agricultural sprays for insecticides and in gasoline blends.[9]

Xylene is primarily used as a solvent, and it can be found in protective coatings, lacquers, enamels, rubber cements and cleaning agents. The three isomers are also used individually as starting materials in the manufacture of various chemicals. For example, o-xylene is used to produce phthalic anhydride, m-xylene to produce isophthalic acid and p-xylene as a precursor of tetraphthalic acid.[10]

In 1983, Canada produced over 400 000 tonnes of both toluene and xylene.[11] Estimates of usage of ethylbenzene and xylene in areas surrounding the Great Lakes Basin were given in a 1981 Annual Report in which human health effects in the Great Lakes area were assessed.[12] The annual use or production of ethylbenzene in Ontario is 200 million kilograms. Ontario uses more than 100 million kilograms of xylene annually.

The alkyl benzenes are recognized primarily as atmospheric pollutants mainly because of their high volatility, but small amounts may enter aquatic and terrestrial systems (e.g., gasoline spills from leaking storage tanks).

Exposure

In a study of 30 potable water treatment plants in Canada, analysis of the raw water showed toluene, ethylbenzene and o-, m- and p-xylenes present in 27, 14 and 7 of the 60 samples, respectively.[13,14] In both the raw and treated water, ethylbenzene and m-xylene were found at concentrations below 0.001 mg/L, whereas the concentration of toluene was 0.002 mg/L in the treated water. In a study of Ontario drinking water, toluene and xylene were found at concentrations ranging from the detection limit of 15 ng/L to 500 ng/L.[15] When drinking water from 12 Great Lakes municipalities was analysed, toluene was detected in five areas (1.0 to 2.8 ng/L) and o- and p-xylene in seven areas (1.1 to 12.0 ng/L total).[16] No values were given for ethylbenzene.

Alkyl benzenes have been measured in ambient air, but there are very few data for indoor air or for food.

Analytical Methods and Treatment Technology

Analysis of toluene, ethylbenzene and the xylenes may be done by a purge and trap gas chromatographic procedure used for the determination of volatile aromatic organic compounds in water.[17] With the use of a photoionization detector, the detection limit for all of the above-mentioned compounds is 0.02 µg/L. The detection limit for confirmation by mass spectrometry is 0.2 µg/L. It is likely that the practical quantitation limit (based on the ability of laboratories to measure these compounds within reasonable limits of precision and accuracy) is about 5 µg/L, as it is for benzene.

Conventional water treatment processes may be partially effective for removing the xylenes from drinking water but ineffective for the removal of toluene or ethylbenzene. Aeration or air stripping is an effective, simple and relatively inexpensive process for removing xylene and other organics from water. However, use of this process transfers the contaminant directly to the air stream. When considering the use of air stripping as a treatment process, it is suggested that careful consideration be given to the overall environmental occurrence, fate, route of exposure and various hazards associated with the chemical.

Aeration appears to offer the best potential for removing ethylbenzene from contaminated water.

Health Effects

The majority of the available information on the chronic toxicity of the alkyl benzenes and xylenes relates to the inhalation route. Some data available on the oral route of exposure lead to the conclusion that these compounds are rapidly absorbed and that the side-chain alkyl groups are rapidly and extensively metabolized by microsomal mixed-function oxidases to water-soluble acids or their conjugates, which are readily excreted via the kidneys.

Rats were given oral gavage doses of 13.6, 136, 408 or 680 mg/kg bw per day of ethylbenzene in olive oil for 130 days of the 182-day test period.[18] No effects were observed in rats given doses of 13.6 and 136 mg/kg bw per day. Increases in liver and kidney weights were reported following oral administration of 408 or 680 mg/kg bw per day. There were also slight histopathological changes at those dose levels. No results of similar experiments involving the oral injection of toluene or the xylenes were found.

Classification and Assessment

From the available information on the toxicology of toluene, ethylbenzene and the xylenes, the exposures or doses related to the induction of central nervous system, respiratory or irritant effects exceed, by several orders of magnitude, the levels known to elicit organoleptic effects. Therefore, these substances have not been classified on the basis of potential health effects.

Aesthetic Considerations

Alexander and co-workers measured aqueous odour and taste thresholds for various chemicals.[19] The odour threshold values were reported as milligrams of compound per litre of odour-free water at 60°C. The authors stated that the odour thresholds measured at 60°C should be applicable to ambient temperature, because the temperature effect appeared to be small. The taste threshold values were reported as milligrams of compound per litre of odour-free water at 40°C.

For toluene, two odour threshold measurements of 0.024 mg/L were reported; for ethylbenzene, two odour threshold measurements of 0.0016 and 0.0032 mg/L (average value 0.0024 mg/L) were reported.

Also for toluene, two taste threshold measurements of 0.12 and 0.16 mg/L (average value 0.14 mg/L) were reported; for ethylbenzene, two taste threshold measurements of 0.064 and 0.08 mg/L (average value 0.072 mg/L) were reported.

For the xylenes, Middleton *et al.* stated that taste and odour could be detected at concentrations ranging from 300 to 1000 ppb (0.3 to 1.0 mg/L).[10]

Rationale

The aesthetic objectives are ≤0.024 mg/L for toluene (the odour threshold cited above); ≤0.0024 mg/L for ethylbenzene (average of the odour thresholds cited above); and ≤0.3 mg/L for total xylenes (the lowest taste and odour threshold cited above).

References

1. U.S. Environmental Protection Agency. Ambient water quality criteria for toluene. Report No. EPA-440/5-80-075, October (1980).

2. American Petroleum Institute. Technical data book — petroleum refining. Division of Refining, New York, NY (1966).

3. Mellan, I. (ed.). Industrial solvents handbook. 2nd edition. Noyes Data Corporation, Park Ridge, NJ (1977).

4. U.S. Environmental Protection Agency. Health assessment document for toluene. Report No. EPA-600/8-82-008, March (1982).

5. Hansch, C. and Leo, A. Substituent constants for correlation analysis in chemistry and biology. John Wiley & Sons, New York, NY (1979).

6. Windholz, M., Budavari, S., Stroumotos, L.Y. and Fertig, M.N. (eds.). Merck index. Merck & Co., Rahway, NJ (1976).

7. National Research Council. The alkyl benzenes. Committee on Alkyl Benzene Derivatives, National Academy Press, Washington, DC (1981).

8. Industrial Environmental Research Laboratory. Multimedia environmental goals for environmental assessment. Report No. PB80-115116, Research Triangle Park, NC, August (1979).

9. U.S. Environmental Protection Agency. Ambient water quality criteria for ethylbenzene. Report No. EPA-440/5-80-048, October (1980).

10. Middleton, F.M., Rosen, A.A. and Burttschell, R.H. Taste and odour research tools for water utilities. J. Am. Water Works Assoc., 50: 21 (1958).

11. Statistics Canada. Publ. No. 5-3304-727, Manufacturing and Primary Industries Division, February (1984).

12. International Joint Commission. Committee on the Assessment of Human Health Effects of Great Lakes Water Quality. 1981 annual report. November (1981).

13. Otson, R., Williams, D.T. and Biggs, D.C. Relationships between raw water quality, treatment and occurrence of organics in Canadian drinking water. Bull. Environ. Contam. Toxicol., 28: 396 (1982).

14. Otson, R., Williams, D.T. and Bothwell, P.D. Volatile organic compounds in water at thirty Canadian potable water treatment facilities. J. Assoc. Off. Anal. Chem., 65(6): 1370 (1982).

15. Smillie, R.D., Sakuma, T. and Duholke, W.K. Low molecular weight aromatic hydrocarbons in drinking water. J. Environ. Sci. Health, A13(2): 187 (1978).

16. Williams, D.T., Nestmann, E.R., Lebel, G.L., Benoit, F.M. and Otson, R. Determination of mutagenic potential and organic contaminants of Great Lakes drinking water. Chemosphere, 11(3): 263 (1982).

17. U.S. Environmental Protection Agency. Method 503.1. Volatile aromatic organic compounds in water by purge and trap gas chromatography. Environmental Monitoring and Support Laboratory, Cincinnati, OH (1985).

18. Wolf, M.A., Rowe, V.K., McCollister, D.D., Hollingsworth, R.L. and Oyen, F. Toxicological studies of certain alkylated benzenes and benzene. Arch. Ind. Health, 14: 387 (1956).

19. Alexander, C., McCarty, W.M., Bartlett, E.A. and Syverud, A.N. Aqueous odour and taste threshold values of industrial chemicals. J. Am. Water Works Assoc., 74: 595 (1982).