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Aqueous Odor and Taste Threshold Values for Products			
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Abstract

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A standard odor calibrating substance, 1-butanol, was used to compare our panel's values with values reported in the literature.

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DESCRIPTIVE SUMMARY WITH CONCLUSIONS: (Include in this space references to data books, and to earlier related reports, patents and publications.)

Data has been generated on odor threshold for 48 compounds and 29 of these [redacted] products have also been evaluated for taste threshold. This information will be valuable in assessing potential loss or spill hazard of the materials during transport or storage.

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INTRODUCTION

Chemicals entering surface water by spill or waste effluents may cause odor and taste problems in surface water supplies. Many industries, especially those involved in food processing, beverage bottling, and pharmaceutical manufacturing, as well as all drinking water supplies, require high quality water essentially free of odor and taste. Odor can be defined as the concentration of material that produces a noticeable response to the testers olfactory system. Taste is much more complicated. The literature reports only four true tastes: sweet, sour, bitter, and salty, but when accompanied with odor the resulting flavor is usually interpreted as taste.

The objective of this study was to generate odor and taste data on products for use in emergency response to a spillage into public waters during transport or storage.

METHODS

Odor threshold values are presented as the least detectable odor observed by panelists and reported as milligrams of compound/liter of water (mg/ℓ) at 60°C. The least detectable taste of compounds in water at 40°C observed by panelists is the taste threshold value. Taste threshold value is reported in milligrams of compound/liter of water (mg/ℓ).

Evaluation of a compound for odor and taste threshold requires special environmental and procedural controls. These studies were conducted by trained panelists in an odor-free room, using odor-free water, colored glassware (to prevent the panelists from being influenced by physical characteristics of the test compound in solution) constant temperature and relative humidity.

A number of methods for evaluating odor and taste threshold have been described in the literature. Most of these methods have been concerned with odor and taste (flavor) in foods (1,2,3,4). There has been considerable data collected on odor values of various compounds in air (5,10).

Odor Threshold

Odor threshold values in this study were obtained using a modification of the ASTM method D-1292 (6). Stock solutions of the compounds were made by dissolving the chemicals in odor-free water. The usual stock solution contained 1 gm of chemical/ℓ of odor-free water. Dilutions were made when the solution was very odoriferous. Smaller samples of the chemical were used for compounds with low solubility.

Using the triangle procedure, the odor thresholds of compounds in this study were determined by comparison with odor-free water. Three 500 mℓ, glass stoppered, dark brown erlenmeyer flasks were used as the testing flasks. A constant temperature of 60°C was maintained using an electric hot plate. The three odor-free flasks containing 250 mℓ of solution were presented to a panelist. Two flasks contained odor-free water and one contained the test compound. The tester would shake the flask, remove the glass stopper and smell the vapors. The starting concentration was usually high enough to detect and characterize the odor. Then, an increase or decrease in concentration was made and the evaluation repeated until the threshold was determined for each panelist. Threshold values were calculated: mℓ of compound stock solution x concentration of stock solution (mg/mℓ) x $\frac{1000\ m\ell}{250\ m\ell}$.

Taste Threshold

Taste thresholds were performed by panelists who made a judgement as to the least detectable concentration of a compound in water that they could taste. This determination was carried out with the same rigorous environmental and procedural control used during the odor threshold evaluation and using a similar technique.

Taste tests were conducted at 40°C, as this is near body temperature and no sensation of hot or cold was encountered. Normally, the taste threshold determination immediately followed the odor test. The panelist was instructed to swirl the flask, take a sample into the mouth, hold for a few seconds and spit it out without swallowing. Response, recording and calculations were made the same as for the odor threshold.

A modification in procedure when testing a very odoriferous compound was necessary. The panelist was instructed to swirl the flask, inhale and hold his breath while going through the taste procedure. The products presented another modification because of their foaming characteristic. The testing flasks were shaken or swirled for the tester by the second panelist to prevent biasing their response.

Odor-Free Room

A special odor-free room was used for testing. The odor-free room was ventilated by air filtered through activated carbon. A constant temperature of 21°C and relative humidity of ∿50% was maintained.

Odor-Free Water

Odor and taste-free water was prepared from raw [redacted] water by slow passage through a column of activated charcoal filter.

Panelists

Panelists chosen for this study were experienced personnel familiar with chemical odors. Therefore, values presented here should reflect this sensitivity. Extraneous odor stimuli were avoided by not using scented soaps, perfumes, cosmetics or after shave lotions. Odor and taste testing is a fatiguing procedure. Panelists were usually exposed to no more than four compounds a day when determining odor and two compounds when both odor and taste were determined.

A calibrating standard odor substance, 1-butanol was used to compare the odor sensitivity of the panel. No standard was included for taste.

The threshold evaluations in this study were usually conducted by two panelists.

RESULTS AND DISCUSSION

People vary greatly as to odor and taste sensitivity. The use of 1-butanol as a calibrating standard for odor threshold was suggested in APHA 1975 (7). Our experienced test panelists were more sensitive to 1-butanol than was reported by other investigators (8,9,10). They reported the odor threshold of 1-butanol in water in a range of 1.0-2.88 ppm, whereas, our panelists were able to detect 0.27 mg/ℓ (0.2-0.4). The data presented here has been developed with standardized and defined procedures. Variations in threshold concentrations reported in the literature can be attributed to various factors including the experimental techniques, the panelists used, the treatment of the data, and the purity of the compounds studied. Most of the compounds studied here were production samples.

Odor threshold values determined for the compounds in this study are presented in Table I.

Taste threshold values are reported in Table II.

Table III contains a summary of data for odor and taste thresholds of chemicals in water available before this report (11).

Our threshold values were obtained at 60°C for odor threshold and 40°C for taste threshold. It has been postulated as to what values might be expected at ambient temperature. Lillard, et al (8) conducted their odor threshold studies at both 60°C and room temperature. They reported that the threshold values obtained at 60°C in most cases did not differ or were higher than those determined at room temperature.

Three compounds were retested for odor threshold using water temperatures of 40°C and 20°C. The results of which are shown in Table V. Extrapolations for these compounds were made using Antoine vapor pressure constants. Comparison of these values is included in Table V.

Extrapolated values in Tables IV and V were calculated from the approximate vapor-liquid-equilibrium equation

$$c'/c = x''/x = (\partial/\partial')(P/P'),$$

where c is concentration, x is mole fraction, and ∂ is the liquid-phase activity coefficient. These symbols refer to the compound in dilute, aqueous solution. P is the vapor pressure of the pure compound. Unprimed symbols refer to 60°C and primed symbols to lower temperatures.

The ratio ∂/∂' was assumed to be unity. This may cause significant error if ∂ changes rapidly with temperature and concentration. The equation involves two additional assumptions: a) that the vapor is an ideal mixture of ideal gases and b) that the mole fraction of compound in the vapor (air-water-compound mixture) at the odor threshold is independent of temperature.

The ratio P/P' was calculated from the Antoine equations in Table IV. These provide a reliable means of interpolating experimental vapor pressures at the desired temperatures. Some high-boiling liquids involve extrapolation which may introduce minor error.

The extrapolated values in Table V show the proper direction of change but the amount is much larger than observed. This discrepancy is presumably due to the approximate vapor-liquid-equilibrium equation used to extrapolate the observed odor thresholds from 60°C to 40° C and 20°C. Detection of odor involves a physiological response and also the physical processes by which molecules pass from the liquid to the nose. Physical factors include not only vapor-liquid equilibrium but also surface concentration, vaporization rate, and vapor transport. These factors are pertinent to other fields: evaporation of contaminants from water (12) and stripping of contaminants from water (13). Research in these fields may suggest a better model for extrapolation of odor thresholds.

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TABLE I

Odor Threshold Values (mg/ℓ) of Various Chemicals in Water at 60°C

Compound	Panelist*	Threshold	Average Threshold	Characteristic odor

Odor Threshold Continued...

TABLE I

Compound	Panelist*	Threshold	Average Threshold	Characteristic odor

TABLE I

Compound	Panelist*	Threshold	Average Threshold	Characteristic odor

Odor Threshold Continued...

TABLE I

Compound	Panelist*	Threshold	Average Threshold	Characteristic odor
[redacted]				
butanol-1	A	0.2	0.27	
[redacted]	B	0.2		
	C	0.4		
[redacted]				

TABLE II

Taste Threshold Values (mg/ℓ) of Various Chemicals in Water at 40°C

Compound	Panelist*	Threshold	Average Threshold	Characteristic odor

Taste Threshold Continued...

TABLE II

Compound	Panelist*	Threshold	Average Threshold	Characteristic odor

TABLE III

10/27/75

SUMMARY OF [redacted]

Expressed in Parts Per Billion

Compound	Odor Threshold	Taste Threshold	Date
Ethylene dichloride	1,800		1/68

TABLE IV

Antoine Vapor Pressure Constants ($\log P_{mm} = A - \frac{B}{t + C}$) (t in °C)

Name	Bruto Formula	A	B	C	t_{760}/°C	Calculated Odor Threshold mg/ℓ 40°C	20°C
[redacted]							
Butanol-1	$C_4H_{10}O$	7.47680	1362.39	178.77	117.66	0.9	3.8
[redacted]							

TABLE V

ODOR THRESHOLD

Experimental Vs. Extrapolation

	mg/ℓ		
Butanol-1	60°C	40°C	20°C
Exp.	0.27	0.3	0.8
Extra.		0.9	3.8

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