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ORIGINAL ARTICLE

Use of *n*-butanol as an odorant to standardize the organoleptic scale of breath odour judges

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OBJECTIVE: The alcohol *n*-butanol has been recommended for use as a standard odorant by various groups for the training or standardization of breath odour judges and sensory evaluation panels. The objective of this study is to assess the use of *n*-butanol as a suitable odorant for organoleptic training of breath judges.

METHODS: One judge with full smell acuity was trained in the method of organoleptic assessment using odorant solutions of main chemical classes (acids, amines, indole and sulphides) with the exception of alcohols. The subject was proficient in scoring odorant solutions, standard gas mixtures and human breath using the Rosenberg 0–5 organoleptic scale. A wide range of *n*-butanol solutions were prepared from 0 to 90 000 ppm and dispensed as replicate 12-ml volumes in Universal bottles (24 ml) leaving a headspace of 12 ml. Sets of odorants were prepared, labelled by code, randomized and presented to the judge in a completely blind fashion. The judge scored each concentration. This process was repeated on 32 occasions over a period of 12 weeks. Mean values of data for each determination for each concentration series were plotted against the log concentrations of odorant. Linear regression slope analysis was used to measure slope, the 95% CI of slope and the scatter of points (R^2 value). Headspace concentrations of odorant were determined using gas chromatography (GC) analysis.

RESULTS: The *n*-butanol regression slope gave a high R^2 value (0.971) and low scatter. However, the data did not correspond to other published work using an ASTM method where the range of recommended butanol concentrations was insufficient at both the high and low ends to determine the top and threshold. Moreover, headspace analysis using GC confirmed the published gas concentrations to be in error by a factor of 100. It was also observed that high concentrations of odorants were irritant causing desensitization if used for prolonged periods.

CONCLUSION: The published method had erroneous headspace calculations listed and *n*-butanol could not be recommended as a training odorant because of its irritancy.

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Keywords: *n*-butanol; organoleptic training; odour judges; organoleptic scale

Introduction

Many compounds have been suggested as being suitable for training and calibrating odour judges. *n*-Butanol has been used previously (ASTM, 1999) as it can be obtained pure, is non-toxic, is stable in air or water and its odour is considered to be not unpleasant. It was important for us at University of the West of England as a centre for organoleptic training to determine the usefulness of *n*-butanol for our own training purposes. Therefore, the objective of our work was simply to assess the use of *n*-butanol as a suitable odorant for use in organoleptic training of breath odour judges.

Material and methods

Choice of judge

One judge with full smell acuity was trained in the method of organoleptic assessment using odorant solutions of all chemical classes (acids, amines, indole and sulphides) with the exception of alcohols. Prior to this study, the judge demonstrated her ability to distinguish odours using the smell identification tests (Sensonics Inc., Haddon Heights, NJ, USA), a method which was employed to detect specific and non-specific anosmia. The subject was proficient in scoring odorant solutions, standard gas mixtures and human breath using the Rosenberg 0–5 organoleptic scale. The judge had gained over 5 years experience of assessment and for the purposes of this work was considered to be the gold standard.

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Odorant preparation and presentation

A wide range of *n*-butanol solutions were prepared from 0 to 90 000 ppm and dispensed as replicate 12-ml volumes in Universal bottles (24 ml) leaving a headspace of 12 ml. Sets of odorants were prepared, labelled by code, randomized and presented to the judge in a completely blind fashion. The judge scored each concentration. This process was repeated on 32 occasions over a period of 12 weeks.

Organoleptic scale

The modified scale of Rosenberg was employed (Greenman *et al*, 2004). The scores are described as: 0 = no odour (below the smell threshold), 1 = barely noticeable odour, 2 = slight odour, 3 = moderate odour, 4 = strong odour, and 5 = extremely strong odour close to saturation.

Gas chromatography analysis of headspace gas concentrations

Headspace concentrations of odorant were determined using gas chromatography (GC) (Hewlett Packard/HP 5890, Palo Alto, CA, USA) with automatic injection of headspace gas (1 ml). Detection was achieved using a hydrogen flame ionization detector.

Calculation of headspace gas concentration from Henry's constant

For the purposes of this work, the dimensionless Henry's law constant at 20°C at 1 atmosphere pressure for *n*-butanol was taken to be 1.1×10^2.

Expression of data

Mean values of data for each determination for each concentration series were plotted against the log concentrations of odorant. Linear regression slope analysis was used to measure slope, the 95% CI of slope and the scatter of points (R^2 value).

Results

The relationship between *n*-butanol concentrations in liquid (water) and the gas phase (12 ml + 12 ml) is shown in Figure 1. This shows both the measured values (by GC analysis) and the theoretical values calculated from Henry's constant. There was close agreement between the theoretical and measured values up to a liquid concentration of 4.0×10^{-1} (mol dm^{-3}). At higher concentrations there was a departure from the linear relationship (because of saturation of the gas phase).

The results from plotting the organoleptic scores against the log concentration of *n*-butanol (in the gas phase) are shown in Figure 2. The regression slope gave a high R^2 value (0.971) and low scatter.

The nominal concentrations for threshold (score 0) to saturation (score 5) is shown in Table 1. This table also shows figures for a recommended method given by an unnamed US-based group on ASTM (1999). There was a wide discrepancy between the two methods. The range of concentrations cited in the recommended method was insufficient at the high end to determine the top of the organoleptic scale and insufficient at the low end to determine threshold. Moreover, the gas concentrations cited in the recommended method were in error by a factor of over a 100-fold compared with both the theoretical values (Henry's constant) and by the practical measures using GC.

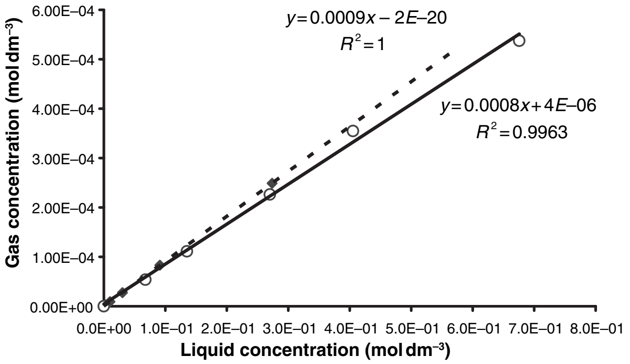

Figure 1 Gas–liquid phase relationship for *n*-butanol; correlation between liquid and gas concentration (mol dm^{-3}). Relationship determined by theory (from Henry's constant) [dotted line]. Relationship determined from GC measurements [solid line with points]

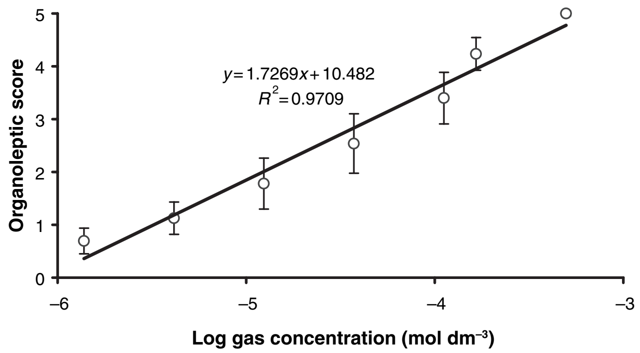

Figure 2 Relationship between organoleptic scores and log gas concentration of *n*-butanol. The error bars show ± s.d. from $n = 32$ at each concentration point

Discussion

The judge reported that high concentrations of odorants were irritant and tiring to the nose. Initial experiments conducted after exposure to the higher concentrations of *n*-butanol, suggested wider scatter in subsequent determinations. However, there are insufficient determinations to characterize this effect in quantitative terms and further work is needed. In conclusion, a previously described US method protocol had erroneous headspace calculations listed and the scale described did not reflect the organoleptic scale of the UK system. This wide discrepancy suggests the need for a more controlled approach to organoleptic training and standardization of

Table 1 Comparison of butanol liquid concentrations (ppm) and concentrations in the gas and liquid phases expressed as mol dm^{-3} with corresponding organoleptic scores for each concentration data from the University of the West of England (UWE) and a US group

Butanol liquid concentration (ppm)	*Equivalent liquid concentration (mol dm^{-3})*	*Equivalent gas concentration (ppm)*		*Equivalent gas concentration (mol dm^{-3})*		*Organoleptic scores*	
		UWE	*US*	*UWE*[a]	*US*[a]	*UWE*	*US*
0	0	0	0	0	0	0	0
10	0.001351	0.0009	–	5.51572×10^{-8}	–	0	–
250	0.033784	0.227273	25	1.37893×10^{-6}	3.380×10^{-4}	1	1
750	0.101351	0.681818	75	4.13679×10^{-6}	1.014×10^{-3}	1	2
2250	0.304054	2.045455	225	1.24104×10^{-5}	3.041×10^{-3}	2	3
6750	0.912162	6.136364	675	3.72311×10^{-5}	9.122×10^{-3}	2.5	4
20 250	2.736486	18.40909	2025	1.11693×10^{-4}	2.736×10^{-2}	3.5	5
40 500	4.054054	36.818	–	2.23386×10^{-4}	–	4	–
81 000	12.16216	73.636	–	4.46772×10^{-4}	–	5	–

[a] Gas concentrations (mol dm^{-3}) based on previously given gas ppm concentrations respectively.

organoleptic malodour judges, in order to reduce inter-judge variations, especially of those from different centres from around the world. Although the magnitude of irritancy that *n*-butanol may cause the nose has not been quantified, it could not be recommended as a training odorant because of its irritant nature.

References

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