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Relationship Between Odour Intensity and Concentration of n-Butanol

J. C. Segura

Alberta Agriculture, Food and Rural Development, Edmonton, AB T6H 5T6

J. J. R. Feddes

Department of Agricultural, Food and Nutritional Science, University of Alberta,
Edmonton, AB T6G 2P5

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Abstract

A study was undertaken to determine the relationship between the concentration of an air n-butanol mixture based on the 8-point odour intensity reference scale (OIRS) assessed by odour sniffers (human odour assessors) and the corresponding n-butanol concentration determined by olfactometry. Odour dispersion models are validated from odour intensity data assessed in the field by odour sniffers. However, the odour intensities provided by odour sniffers do not correlate well with the predicted values by dispersion models. It is possible that the odour sniffers training protocol is a factor in the poor dispersion model correlation observed. An important assumption in the intensity training process was the theoretical, Henry's Law, n-butanol concentrations in air for the OIRS n-butanol solution concentrations. A calibration technique was followed to determine the true relationship between the 8-point OIRS n-butanol solutions in jars and their respective n-butanol concentrations in air. The technique developed a relationship between the 8-point OIRS intensities and n-butanol concentrations in air that has not been reported previously. The training required by the odour sniffer using the n-butanol in jars can be replaced by the protocol described in this research using an olfactometer as a more reliable and accurate intensity training instrument. The odour concentration-intensity relationship for n-butanol was found to be different from odour concentration-intensity relationships for animal odours.

Keywords. Odour, intensity, concentration, n-butanol, olfactometry.

INTRODUCTION

Odour emissions from livestock operations and downwind odour intensity values are a major component of calibrating and validating odour dispersion models. To obtain these values, an odour intensity referencing scale (OIRS) is used which can have 5, 8, 10 or 12 points of intensity, and the values are transformed using various models into detection threshold odour units or odour concentrations (OU/m^3). The OIRS is defined in ASTM E544 (1999) and reported by McGinley (2000).

Substantial discrepancies between transformed intensity values provided by a group of odour sniffers (Nasal RangersTM) and the predicted values by a dispersion model were found during an odour dispersion modeling study (Scott, 2003). The differences could occur due to the small quantity of measurements collected by the group of sniffers. Scott indicates that models developed by Zhang *et al.*, (2002) and Zhu *et al.*, (2000) were used to transform the collected odour intensities by the trained odour sniffers into concentrations. Other reasons for the differences might be the interpretation of the olfactometry results, changes in the n-butanol concentrations during training, differences in the nature of odour (animal vs. chemical), sniffer selection criterion (i.e. age, socio-cultural background) and sniffer capabilities to recognize and differentiate agricultural odours.

An important aspect in the training process of odour sniffers is to know if the specified concentration of the OIRS is accurate. During the odour sniffer training for this project, it was hypothesized that the air surrounding the person's nose was entrained into the headspace of the container containing the n-butanol liquid, which led to a dilution of the specified odorant thus changing the expected original concentration. Also, dilution occurred the moment the lid of the container was opened before the odour sniffer had a chance to smell the solution.

It was also observed that no data points were presented below $60 \text{ OU}/\text{m}^3$, for the development of the predicted model by Zhu (2000), thus the regression equation was extrapolated to convert the low odour intensity measurements into odour concentrations. This suggests that more research is required to identify the relationship between odour intensity and the corresponding concentration (or detection threshold) of weaker odours.

The present study was undertaken to understand the relationship between the concentration in non diluted air of n-butanol OIRS (static scale) detected by odour sniffers during training and the corresponding diluted concentration during olfactometry (dynamic scale).

BACKGROUND

An odour dispersion modeling study was conducted as a component of a main project "Development of a Scientific Siting Tool & Odour Monitoring Procedures for Alberta Livestock Producers". To accomplish the task the University of Alberta, Alberta Agriculture, Food and Rural Development and Alberta Research Council joined a research group called the Odour Control Initiative

(OCI). A component of this project was to collect odour concentrations downstream from a hog facility by trained odour sniffers. The data collected were used to calibrate/validate an odour dispersion model. Equations developed by Zhang *et al.* (2002) and Zhu *et al.* (2000) to transform the odour sniffers intensity readings (OIRS) into concentration (OU/m^3) were applied. These concentration values were compared with the predicted values using an odour dispersion simulation program Industrial Source Complex (ISC-View, Version 4.8. Lakes Environmental, Waterloo, ON). This model calculates the concentrations downwind from a CFO and should match the concentrations perceived by the odour sniffer at the same locations.

The results showed that the levels provided by odour sniffers in this project were widely divergent from those predicted by the model. It is important to note that the Zhang *et al.*, (2002) and Zhu *et al.*, (2000) models were developed from livestock odour sources. To develop their models, Zhang *et al.*, (2002) and Zhu *et al.*, (2000) both used the expertise of trained odour sniffers, as in this project, but it is possible that variation in the training protocol is a factor in the different results observed.

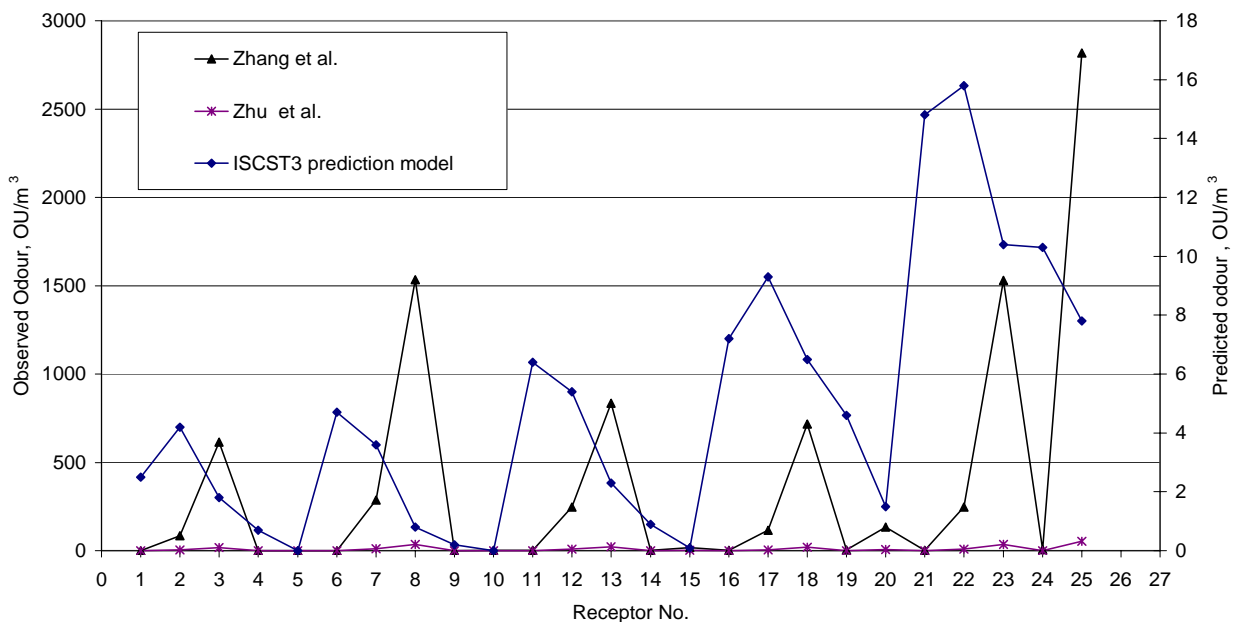


Figure 1. Comparison between the odour intensities recorded by odour sniffers downwind from a CFO (day 266) and the predicted concentration values by the ISC-View dispersion model found by applying Zhang *et al.* (2002) and Zhu *et al.* (2000) intensity – concentration equations. (D. Scott, Personal communication, 2003)

OBJECTIVE

Determine the relationship between the n-butanol vapor concentration in air (ppm) (static scale method, 8-point OIRS) detected by odour sniffers from the headspace of a 60-mL training jar and the corresponding n-butanol concentration (OU/m^3) determined by an olfactometer (dynamic scale method).

METHODOLOGY

Liquid 1-butanol 99.4 mol % purity was used for the preparation of 8 solutions in distilled water. The solutions were utilized during the sniffers training session as the 8-point OIRS. A certified reference material of n-butanol (40 ppm and 200 ppm) in nitrogen was used as the reference and main odorant to be used during olfactometry CEN (2003).

This project was divided in two experimental phases as follows:

Part A

Part A was conducted first. A group of odour sniffers were trained using an adapted static scale method by St. Croix Sensory (2000) and Feddes (2004), following the standard practice ASTM –E 544-99. The OIRS 8-point scale of 1-butanol, 30-mL solutions in 60-mL jars, was presented to the odour sniffers for a minimum of one week prior to the panel sessions. A dynamic triangular forced-choice olfactometer, constructed according to CEN 13725 (2003) standards was used for this section of the project (Feddes, 2000). The n-butanol (air) sources were diluted and presented to the odour sniffers without forcing them to make a choice meaning the sample was presented constantly. The odour sniffer sniffed the port air sample and recorded the intensity of the sample.

Before each olfactometry panel session, three training jars were selected at random from a set of 18 jars (0-8 OIRS) to test and select the most accurate odour sniffers. Four panel sessions using n-butanol as an odour source were conducted in order to match unknown dilutions of n-butanol with their corresponding 8-point scale as estimated by the odour sniffers.

An in-house test was conducted in order to define the approximate minimum and maximum concentrations of n-butanol (ppm) required for the study. The different dilutions were found by selecting at random from a predetermined scale created during an in-house test. The different dilutions were found based on an n-butanol scale with geometric progression ratios of 1.5 and 2. The dilutions selected ranged between 0.014 and 5 ppm of n-butanol in air. During sessions 1 and 2, the first sample was the lowest concentration and subsequent samples progressed to higher concentrations. Each odour sniffer assessed (matched) the concentration with the 8-point reference scale of n-butanol. During sessions 4, 18 dilutions were presented at random. From these results a range of expected concentrations (n-butanol on ppm) was determined and used to define an equation that would correspond the concentrations to intensity (8-point scale).

During panel 1, the n-butanol concentrations were presented in ascending manner at 7 second intervals to the odour sniffers. It was determined during panel 1 that the odour sniffer did not have enough time to assess the odour sample (n-butanol dilution). Consequently, the sniffing time was increased to 10 seconds for the remaining three panel sessions. During all four panels 2 min were provided between samples for odour sniffer's nose to rest.

A minimum of two random fresh air (or blanks) were presented between n-butanol dilutions during the panels, to prevent saturation (sensory fatigue). The resulting values, after finding the corresponding 8 dilutions (ppm) with the 8-point n-butanol scale, were used during the odour panels in part B of this project.

Part B

The olfactometer panelists (not odour sniffers) were presented with multiple samples of the 8 dilutions (ppm) of n-butanol corresponding to those that were found in part A of this study. The eight intensities of n-butanol concentrations (premixed in air and injected in Tedlar® bags) were randomly presented following the normal olfactometry protocol, using the dynamic triangular forced-choice methodology. However, after the first panel, it was found that the odour (n-butanol) concentrations corresponding to 1-5 of the n-butanol scale were similar to or below the lower detection level (LDL) of a new, unused Tedlar® sampling bag. Parker et al. (2003) and Feddes (2004) defined the background odour of a new Tedlar bag in a range from 20 to 60 OU/m³ and from 7 to 70 OU/m³, respectively, measured by detection threshold (DT) using olfactometry. For this reason, the following two panel sessions were divided into two groups. In one group the samples were pre-mixed and presented from bags and in the second group the samples were presented from the n-butanol tank using the olfactometer (gas blending system). The samples presented directly from the tank were the lower intensities (levels 1-4) and the samples presented from bags were the higher intensities (levels 5-8). During panel sessions, random fresh air blanks were given between n-butanol samples 5 to 8 to prevent saturation (sensory fatigue).

The n-butanol concentrations in OU/m³ found during standard olfactometry were correlated with the intensity (air concentrations in ppm) of n-butanol found by the odour sniffers in part A.

RESULTS

Part A

During four panel sessions different concentrations of n-butanol were presented to a group of 8 odour sniffers trained on an 8-point OIRS using. After collecting the values from each panel, an average of the intensities (0 to 8) for each concentration was transformed into a logarithmic form in order to find a linear relationship among all four panels. All the transformed values from the four panels are shown in Figure 2. The *x* axis represents the different n-butanol concentrations presented to the odour sniffers and the *y* axis values correspond to the matching 8-point OIRS given by the odour sniffers.

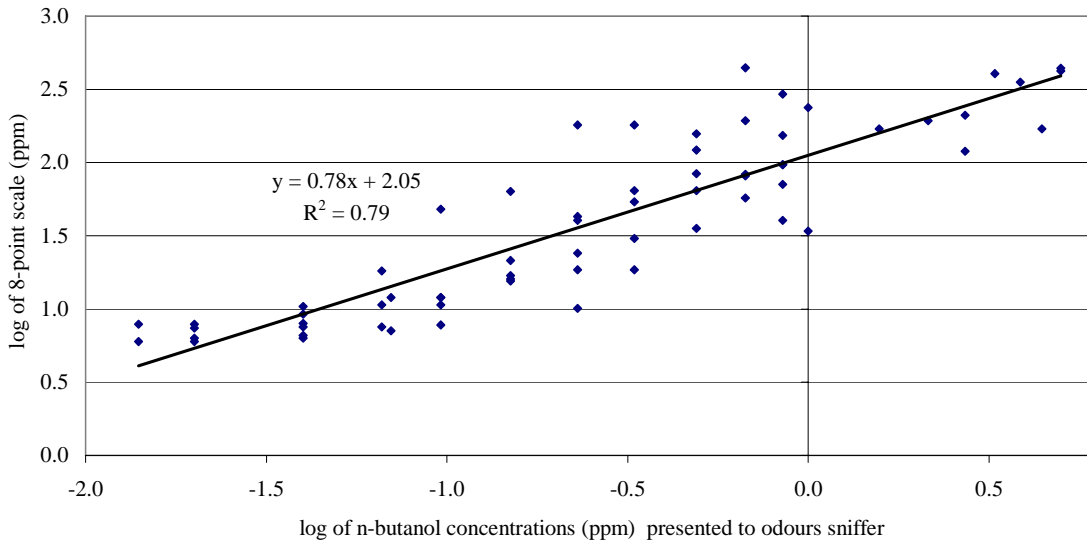


Figure 2. Part A: Relationship between the log of the n-butanol (ppm) concentrations presented to the odour sniffers and its corresponding matched values on the log of the 8-point OIRS.

The equation for part A is presented in Figure 2. It correlated the reported n-butanol concentration in the headspace with the equivalent blended concentration values (ppm) presented to the odour sniffers via olfactometer(i.e. blending system).

The final equation from part A of this study is:

$$\begin{aligned} \text{Log (y)} &= 0.78 \text{ Log (x)} + 2.05 & (1) \\ R^2 &= 0.79 \end{aligned}$$

Where:

y: Log of the 8-point scale n-butanol concentrations in air(ppm), and

x: Log of n-butanol concentrations in air(ppm) presented to the odour sniffers.

Using equation (1), the calibrated n-butanol concentration values that corresponded with the theoretical 8-point OIRS n-butanol concentrations are shown in Table 1. These values were used in Part B to confirm the theoretical threshold detection values calculated based on n-butanol's detection threshold of 40ppb(OU/m³). The lower concentrations were found to be similar to the definition of the accepted reference for the European odour unit concentration of one European Reference Odour Mass unit EROM (40 ppb) (CEN, 2000). This demonstrates that the olfactometer panelists were detecting in the range 20 to 80 ppb n-butanol as required by the European standards (CEN, 2000).

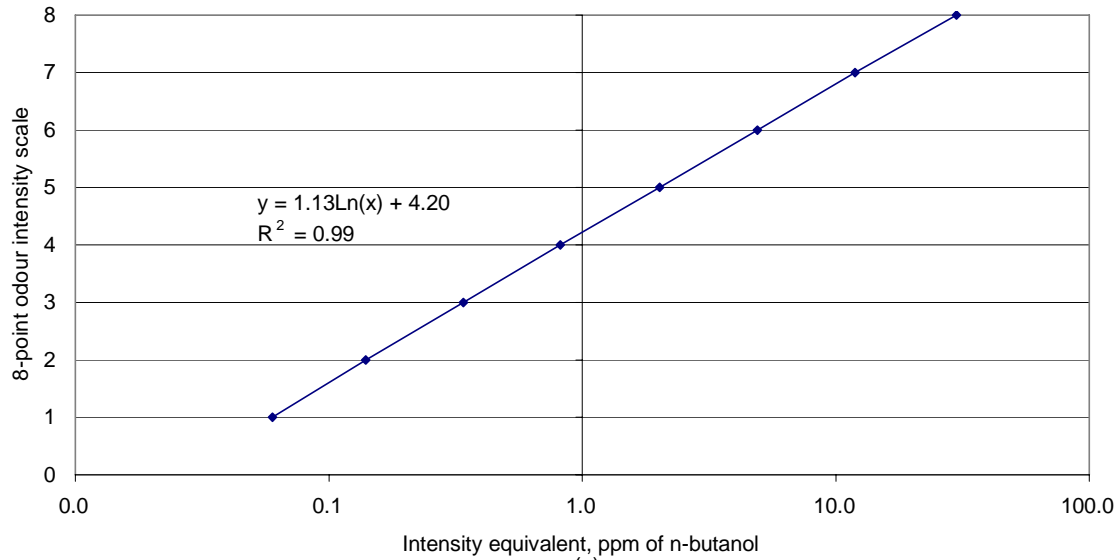


Figure 3. Logarithmic relationship of n-butanol (ppm) concentrations determined in part A by odour sniffers and its corresponding concentration values in the 8-point referencing scale in ppm.

The results from Part A also showed that the technique of training with jars is reliable or consistent in calibrating odour sniffers for detecting n-butanol. That was demonstrated by the high correlation coefficient (R^2) of 0.79 from Equation (1). Figure 3 shows the use of equation (1) to illustrate the calibrated relationship between the log of the 8 point OIRS n-butanol concentrations and the corresponding intensity levels in the 8 point OIRS. For example, the transformation for level 1(y in equation (1)) will be $\log 12 \text{ (ppm)} = 1.08$. Replacing 1.08 on equation 1 and solving $x = -1.24$, and transforming by 10^x the resultant value is 0.06 ppm (Table 1).

Table 1. Relationship of the 8-point scale of n-butanol in air and its corresponding concentrations using olfactometry and the theoretical concentrations based on the definition of one European odour unit (40 ppb or one EROM).

^a Level	^b 8-point n-butanol scale in air (ppm)	^c Part A n-butanol intensities ppm in air	Theoretical concentration OU/m ³	^d Part B Measured concentrations OU/m ³
1	12	0.06	2	2
2	24	0.14	4	5
3	48	0.34	9	12
4	96	0.82	21	26
5	194	2.02	51	57
6	388	4.91	123	128
7	775	11.9	298	286
8	1550	29.0	724	637

^a8-point n-butanol intensity referencing scale (OIRS)

^bn-butanol concentration in air based on ASTM Standard E:544-99

^cIntensities found applying Equation (1).

^dConcentrations found applying Equation (2) using the levels of the 8-point OIRS.

Part B

The results from Part B confirmed that equation (1) is reliable. To verify this, the intensities of n-butanol found in Part A were divided by 40 ppb (0.040 $\mu\text{mol}/\text{mol}$) of n-butanol as defined by one EROM odour unit CEN (2000). The output values matched the concentration of the 8-point scale OIRS values in ppm divided by one EROM. The theoretical values are included in Table 1 and graphed in Figure 4.

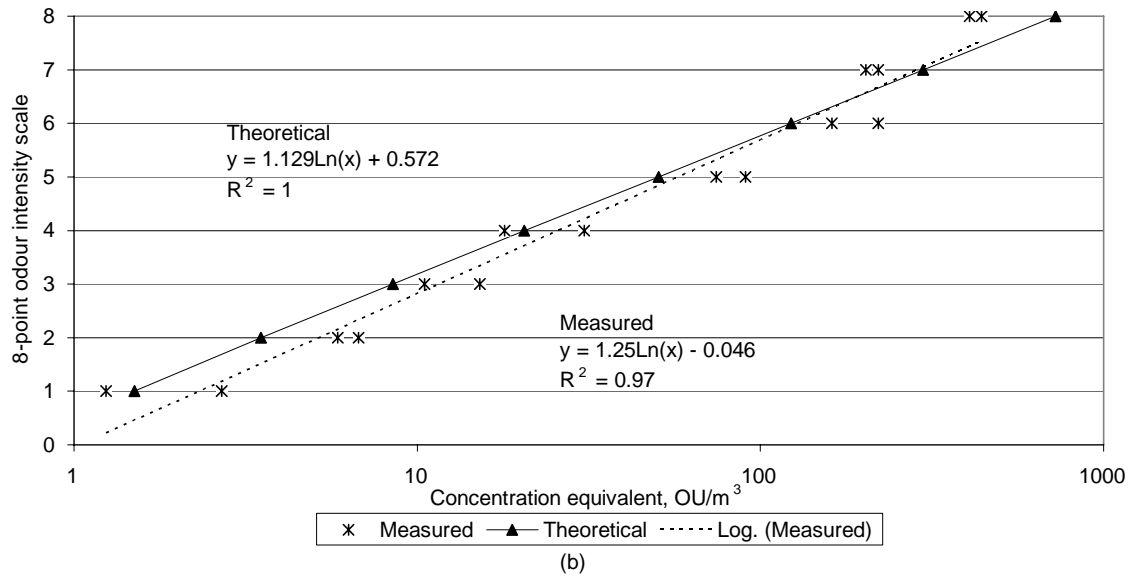


Figure 4. Relationship between intensities found in part A and its corresponding concentrations measured by the panelists.

In Figure 4 the relationship between intensity (odour sniffers) and concentration (olfactometry) is shown in equation 2:

$$I = 1.25 \ln(C) - 0.046 \quad (2)$$

where:

I = odour intensity expressed as ppm of n-butanol in air, and

C = odour concentration in OU/m^3 .

The theoretical curve presented in Figure 4 is the comparison between the current prediction equation (2) and the ASTM n-butanol scale transformed to concentration using the definition value for one odour unit (OU/m^3). Equation 2 has the form of a mathematical model known as the Weber-Fechner model that is commonly used to represent odours intensity-concentration relationships. Nicolai et al. (2000), demonstrate that the Weber-Fechner and Stevens appears to be the best fitting models to describe the intensity-concentration relationship for livestock odours (swine buildings) between <100 and 500 OU. Similarly Zhang et al. (2002) reported that both Weber-Fechner and Stevens models describe adequately

the relationship between odour concentration measured by olfactometry and odour intensity assessed by odour sniffers using the 8-point OIRS . Guo et al. (2001) also reported that the Weber-Fechner model provided the best fit to their experimental data for swine and cattle odours.

In order to compare the current model with Nicolai et al. (2000), Guo et al. (2001), Zhang et al. (2002) and Zhu (2000) the intensity levels were converted to equivalent n-butanol concentration in air corresponding to the 5-point OIRS (Figure 5). The relationship between the n-butanol intensity and its concentration was logarithmic. In Figure 5, the results are presented using the Stevens model. Equations 3, 4 and 5 describe the best fit as follows:

$$\ln (y) = 0.897 \ln (x) + \ln (5.167) \quad (3)$$

or similarly $\ln (I) = k_1 \ln (C) + \ln (K_2) \quad (4)$

where:

I = n-butanol (odour) intensity expressed in ppm.

C = n-butanol (odour) concentration (OU/m³), and

k_1, k_2 constants.

Equation 4 can be transformed to power equation as:

$$I = k_2 C^{k_1} \quad (5)$$

The coefficient of determination was (R^2) 0.96 which is very similar to using the Weber-Fechner model (0.97). In Figure 5, the four different models based on livestock odours presented higher odours concentrations at equal intensities in comparison to the n-butanol model. This suggests that if an odour sniffer predicts an intensity based on n-butanol its corresponding concentration for a livestock odour is going to be always higher than the corresponding concentration for n-butanol.

In other words the odour intensity of n-butanol can represent multiple intensities of livestock odours rather than a single value, however their concentrations will be different creating skewed results when a dispersion model is applied. Furthermore Guo et al., (2001) stressed that each odor intensity level in the OIRS covers a range of odours instead of a single value.

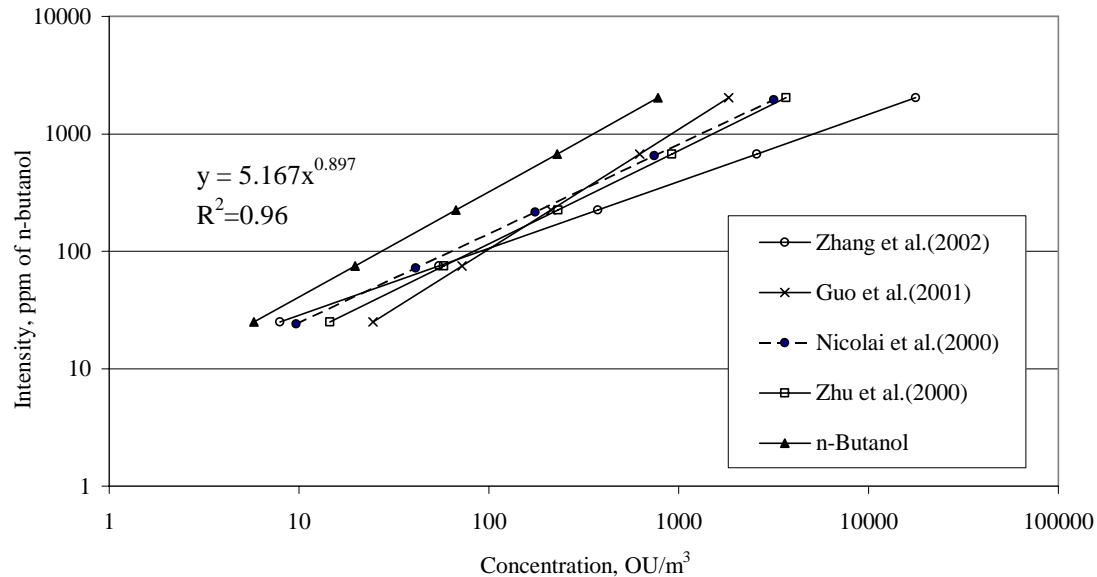


Figure 5. Comparisons between five prediction models using the 5-point intensity referencing scale of n-butanol in air.

CONCLUSIONS

A relationship was found between the n-butanol intensities in air (defined by the ASTM standard E 544-99) and the concentration following the definition of one EROM. The technique developed a relationship among low intensities and concentrations that have not been previously reported.

The training required by the odour sniffers, the n-butanol in jars, can be replaced by the protocol described in this research using an olfactometer. This instrument has been shown to be reliable and accurate. Furthermore, the protocol followed in the project can be slightly modified if the type of gas used for the training is replaced by an artificial livestock odour (ALO) thus making the training system more odour realistic.

This research also demonstrated that the odour concentration-intensity relationship for n-butanol is different from odour concentration-intensity relationships for animal odours. This shows that n-butanol is not a reliable reference odour for livestock odours.

RECOMMENDATIONS

During an in-house test, humidity of the sample can be a factor in the way the n-butanol is perceived as an odour. It is recommended that a project be conducted to determine the importance of the sample moisture content.

It is also recommended when odour intensity-concentration data is required for odour dispersion models, artificial livestock odours should be used rather than n-butanol as a training tool in order to relate

odour sniffers intensity measurements in the field and the concentration of the odour sample from the source to be analyzed.

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