CHEMICAL ENGINEERING TRANSACTIONS
VOL. 54, 2016

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.aidic.it/cet

Guest Editors: Selena Sironi, Laura Capelli

ISBN 978-88-95608-45-7; **ISSN** 2283-9216

Determination of the Odour Concentration and Odour Intensity of a Mixture of Odorous Substances by Chemical Concentrations: a Comparison of Methods

Chuandong Wu[a], Jiemin Liu[a,*], Peng Zhao[b], Martin Piringer[c], Günther Schauberger[d]

[a]School of Chemistry and Biological Engineering, University of Science and Technology Beijing, Beijing, China,
[b]Key Laboratory of Occupational Health and Safety, Beijing Municipal Institute of Labor Protection, Beijing, China;
[c]Environmental Meteorology, Central Institute of Meteorology and Geodynamics, Vienna, Austria;
[d]WG Environmental Health, Unit for Physiology and Biophysics, University of Veterinary Medicine, Vienna, Austria.
liujm@ustb.edu.cn

The assessment of the odour concentration of a mixture of odorous substances is a long lasting problem. Due to the fact that the concentration measurements of chemical substances can be done on a continuous basis, these empirical data are often used to assess the odour concentration of the mixture of these compounds as a substitute of direct odour measurements. Several concepts with increasing complexity are in use for this purpose. Four methods – direct use of measured concentrations, the sum of the odour activity value *SOAV*, the sum of the odour intensities *SOI* and the equivalent odour concentration *EOC* - to convert the concentrations of single substances to the odour concentrations and odour intensities of an odorous mixture are investigated. The methods are compared with olfactometric measurements of seven substances as well as their mixtures. The results indicate that the *SOI* and *EOC* conversion methods deliver reliable values. These two methods use not only the odour threshold concentration but also the slope of the Weber-Fechner law. Due to the fact that no additional olfactometric measurements are necessary, they fulfil the criteria of an objective conversion.
KEYWORDS: Odour concentration, odour intensity, odour activity value, equivalent odour concentration, odorous mixture

1. Introduction

For environmental odour, it is difficult to realise continuous odour measurements for the emission concentration as well as for the ambient concentration in the vicinity of an odour source. These olfactometric measurements are expensive, they can only be done discontinuously, and in many cases only the emission concentration can be measured, because ambient concentrations are often too low to get reliable results. In many cases such odour measurements are substituted by concentration measurements of odorous substances.

The conversion methods which are used to transform the concentration into odour concentration or odour intensity are presented and evaluated by olfactometric measurements. For this conversion several concepts are in use. The simplest approach is the direct use of the concentration of a single substance (e.g. H_2S (Gostelow and Parsons, 2000; Gostelow *et al.*, 2001; Dincer and Muezzinoglu, 2007)) or a group of substances (e.g. VOC concentrations (Capelli *et al.*, 2013)) as a surrogate of the odour concertation using a regression analysis. The second concept called odour activity value *OAV* is based on the normalisation of the concentration C by the odour threshold concentration C_{OT}. If more than one substance is involved, then the sum of the individual *OAVs* is used. This value is called sum of the odour activity values *SOAV* (Parker *et al.*, 2012; Capelli *et al.*, 2013). For a more sophisticated conversion of the concentrations of odorous substances into odour concentrations, we use not only the odour threshold concentration but also the slope of the relationship between odour concentration and odour intensity. Using these parameters, two conversion methods are possible: the sum of the odour intensity *SOI,* which was introduced by Kim and Park (2008) developed for the air quality assessment program in Korea, and the concept of the equivalent odour concentration *EOC* by Wu *et al.* (2016). The conversion from the chemical concentration of single substances to the odour concentrations and odour intensities of an odorous mixture using the four methods is the central topic of this paper. The ability of the four conversion methods to produce reliable odour concentrations is investigated here by comparing them with olfactometric odour concentration measurements; also the odour intensities will be compared. These measurements are described in detail by Wu *et al.* (2016).

2. Materials And Methods

Conversion Methods

Chemical concentration *C*

The simplest approach is the direct use of the concentration *C* of a single substance. The sum of the concentration values is then used as a surrogate for the measured odour concentration C_{OD}. The odour concentration is then calculated by Eq(1)

$$C_{OD}{}^{C} = k_c \sum C_i / m_{OD,0} \tag{1}$$

by using the specific odour mass set to unity $m_{OD,0}$ = 1 mg ou^{-1} to reach a proper measuring unit of the odour concentration (ou_E m^{-3}).

Odour activity value *OAV*

The odour activity value *OAV* is based on the normalisation of the individual concentration of an odorous chemical substance C_i (µg m^{-3}) by the odour concentration threshold $C_{OT,i}$ (µg m^{-3}) with $OAV_i = C_i / C_{OT,i}$. The *OAV* of entire mixture is then calculated by the sum of the individual odour activity values as shown in Eq(2)

$$SOAV = \sum OAV_i \tag{2}$$

Even if the *SOAV* is a dimensionless number, it is often interpreted as an odour concentration (e.g. Wenjing *et al.* (2015), Capelli *et al.* (2008)), called theoretical odour concentration. Therefore we suggest to use the specific odour mass of an individual substance $m_{OD,i}$, which is based on the odour concentration threshold $C_{OT,i}$, to overcome this problem. The related odour intensity OI^{SOAV} is the calculated by OI^{SOAV} = log *SOAV* + 0.5.

Sum of the odour intensities *SOI*

A more sophisticated conversion is using not only the odour threshold concentrations of individual substances but also the slope *k* of the odour intensity - odour concentration relationship (Kim and Park, 2008). The *SOI* is using the odour threshold concentration $C_{OT,i}$ (respectively the derived specific odour mass $m_{OD,i}$) and the odour intensity OI_i calculated by the Weber-Fechner law for each single substance Eq(3).

$$SOI = \log \sum 10^{OI_i} \tag{3}$$

The backward calculation of the odour intensity C_{OD}^{SOI} is done for a selected substance *j* by the Weber-Fechner law (Kim, 2010).

Equivalent odour concentration *EOC*

The concept of the equivalent odour concentration *EOC* is based on the sensitivity of the human nose to a certain odorous substance. The equivalent odour concentration EOC_j related to one selected substance *j* of the mixture can be calculated according to Eq(4).

$$EOC_j = \sum 10^{\frac{k_i}{k_j} \log C_{OD,i}} \tag{4}$$

which corresponds to an odour concentration. The odour intensity of this odorous mixture is then calculated by the Weber-Fechner law with Eq(5).

$$OI^{EOC_j} = k_j \log EOC_j + 0.5 \tag{5}$$

The EOC_j of a selected substance *j* represents the odour concentration of the selected substance *j* which is necessary to perceive the odour concentration of the entire mixture of substances Wu *et al.* (2016).

Chemical substances and olfactometric measurements

In total, 24 binary mixtures of Ethyl acetate and the other six substances were prepared for this investigation. The odour concentration $C_{OD}{}^{olf}$ and the odour intensity of the 23 binary mixtures (one mixture had to be eliminated) of Ethyl acetate and the other six substances and the 5 mixtures of all the seven substances were measured by dynamic olfactometry in the way as it was done with the pure substances. The olfactometric measurements are described by Wu *et al.* (2016).

3. Results and Discussion

For the seven substances the odour threshold concentration C_{OT} (mg m^{-3}), the derived specific odour mass m_{OD} (mg ou$_E^{-1}$), and the slope *k* of the Weber-Fechner law were measured. In Fig. 1, the relationship between the measured odour concentrations C_{OD}^{olf} and the odour intensities OI^{olf} for the single substances as well as the fitted Weber-Fechner law are shown. The statistical details for the regression can be found in Wu *et al.* (2016).

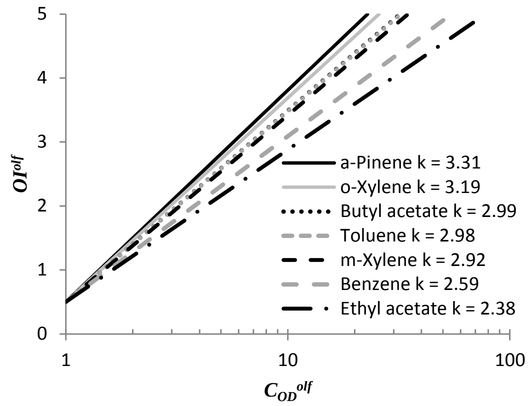

Fig. 1 Relationship between odour intensity OI^{olf} and odour concentration C_{OD}^{olf} (ou$_E$ m^{-3}) and the fitted Weber-Fechner law $OI = k \log C_{OD} + 0.5$ for seven odorous monomolecular substances.

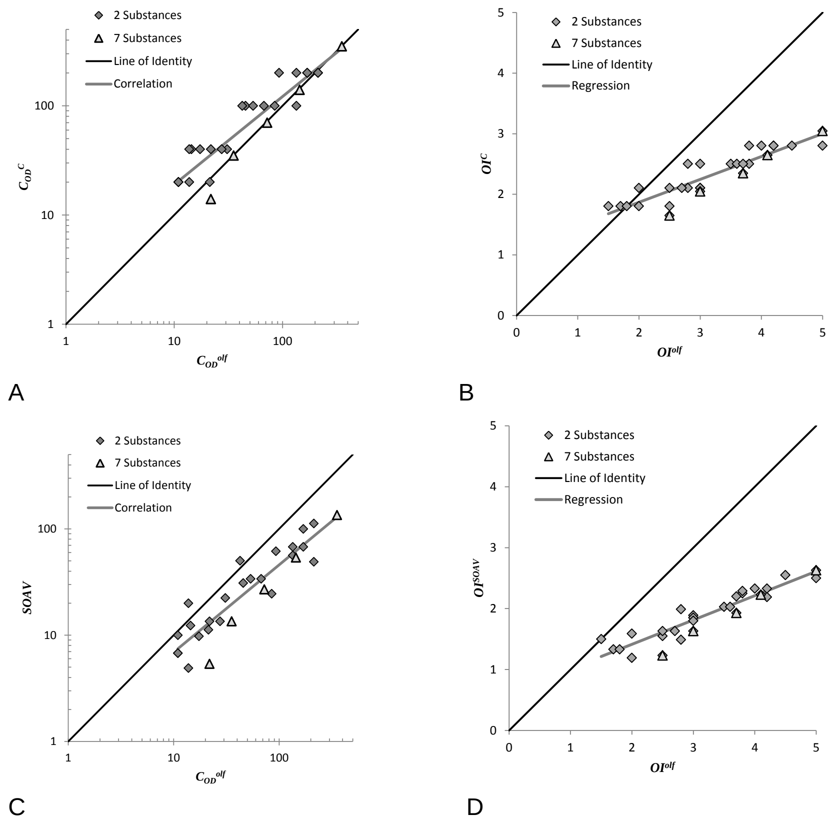

Fig. 2 Comparison of the converted odour concentrations C_{OD}^{C} (A) and SOAV (C) with C_{OD}^{olf} (ou$_E$ m^{-3}) and the converted odour intensities OI^{C} (B) and OI^{SOAV} (D) with the OI^{olf} for the 23 binary mixtures and the 5 mixtures of all seven substances.

The converted odour concentrations and odour intensities from the first two methods show the weakest quality (Fig. 2). These conversion methods will not provide odour intensities which are close to those measured by the olfactometer. Instead, the odour intensities are severely under-estimated.
The odour concentration, calculated by the *SOI* (Fig. A), shows a good correspondence with the line of identity with a slope of 0.9471. The converted odour concentration underestimates the measured odour concentration by about 37%. This under-estimation is even more pronounced for the mixtures of the seven substances. The regression line for the odour intensity shows a good agreement with the line of identity (Fig. B). The slope of the linear regression is 1.12 which results in an overestimation of about 0.5 grades for a high odour intensity of grade 5.
The equivalent odour concentration *EOC* shows a slope of 0.9688 which is close to the line of identity with a weak underestimation of about 13% (Fig. C). The regression line of the resulting odour intensities OI^{EOC} lies parallel to the line of identity with a slope of 1.14 and an overestimation of about 0.6 grades of the 5 grade intensity scale (Fig. 4D).
The last two conversion methods, *SOI* and *EOC,* yield the best results. The regression lines for the odour intensity show a good agreement with the line of identity. Therefore an additional calibration to adapt the slope to the line of identity is not needed.

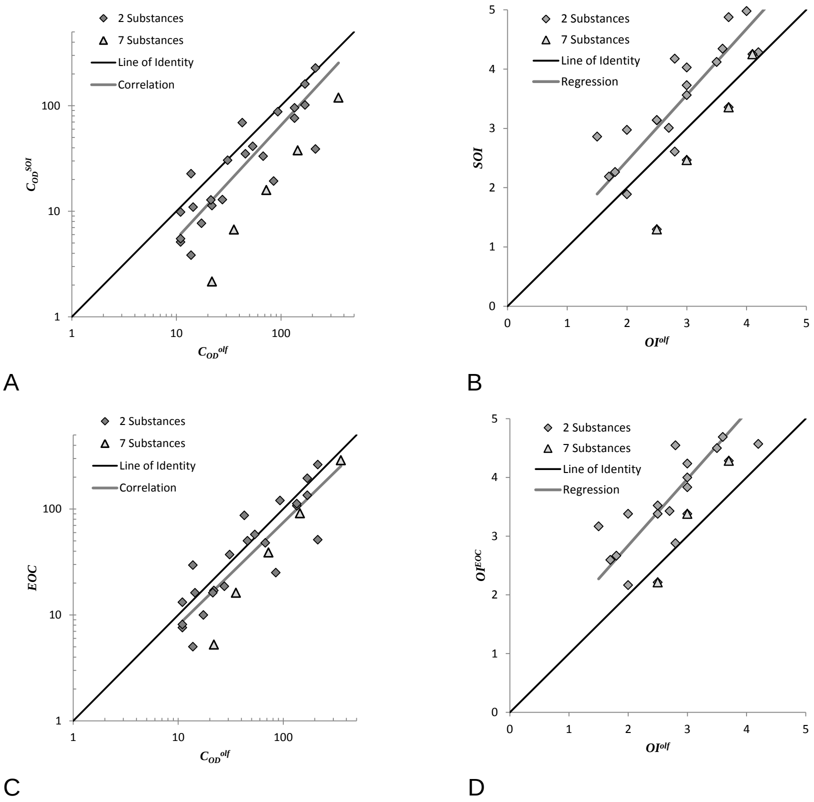

Fig. 3 Comparison of the converted odour concentrations C_{OD}^{SOI} (A) and EOC (B) with C_{OD}^{olf} (ou_E m^{-3}) and the converted odour intensities SOI (C) and OI^{EOC} (D) with the OI^{olf} for the 23 binary mixtures and the 5 mixtures of all seven substances.

In Fig. 4, the *EOC* conversion method is demonstrated with a mixture of two substances Substance α has a steeper slope of k_α = 1.2 than substance β with k_β = 0.8. The calculation of the equivalent odour concentration can be done either related to substance α (EOC_α) or related to substance β (EOC_β). For both substances, the odour concentration is assumed with 100 ou m^{-3}.
Substance α shows a higher perception sensitivity, which is shown by a steeper slope k_α = 1.2 compared to substance β with k_β = 0.8. This means that the equivalent odour concentration for the more odorous substance will result in a lower value of EOC_α = 122 ou m^{-3} compared to the sum of the two odour concentrations $C_{OD,\alpha}$ + $C_{OD,\beta}$ = 200 ou m^{-3} . This means that a concentration of 122 ou m^{-3} of substance α will evoke the same odour intensity as the mixture of the two substances.

For the less odorous substance β it is the other way round. For this substance, a higher equivalent odour concentration EOC_β = 1100 ou m^{-3} is needed to cause the same odour intensity as the mixture of the two substances.

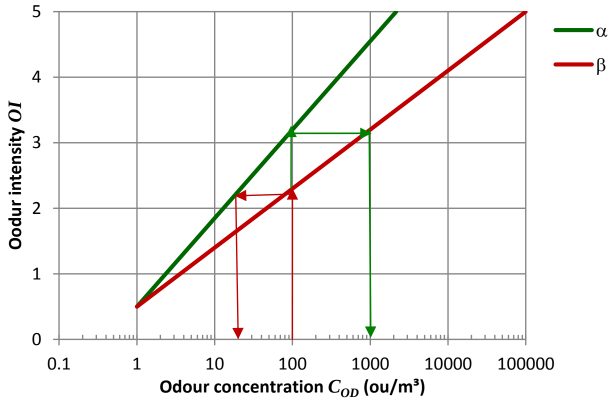

Fig. 4 Example for the equivalent odour concentration EOC for a mixture of two substances. Odour concentration of substance α is $C_{OD,\alpha}$ = 100 ou m^{-3}, for substance β $C_{OD,\beta}$ = 100 ou m^{-3}. The equivalent odour concentration related to substance α will result in EOC_α = 100 ou m^{-3} + 22 ou m^{-3} = 122 ou m^{-3} (shown in red). The equivalent odour concentration related to substance β will result in EOC_β = 1000 ou m^{-3} + 100 ou m^{-3} = 1100 ou m^{-3} (shown in green). For the two substances the Weber-Fechner slope was assumed by k_α = 1.2 and k_β = 0.8.

4. Conclusions

All the discussed concepts are based on the working hypothesis that the mixture of odorous substances behaves additively, which is only a rough estimate (Thomas-Danguin et al., 2014). This means that no interactions between the substances take place. Then the calculated odour concentration CODtheo (called theoretical odour concentration by Capelli et al. (2008)), calculated by the *OAV*, the *SOI* or the *EOC* methods, and the odour concentration measured by an olfactometer C_{OD}^{olf} lie on the line of identity, and $C_{OD}^{olf} = C_{O}^{thef}$.
Beside the odour concentration also the hedonic tone can be influenced by the interactions of several substances. However, there are exceptions where odorants with high *OAV*s are suppressed in the aroma and compounds, whereas lower *OAV*s are important contributors. In general, a mixture is called homogeneous when a new single odour is perceived from the mixture or heterogeneous when several odours can be identified from this mixture.

Acknowledgments

This work was jointly supported by the National Natural Science Foundation of China (Nos. 21277011, 21407008 and 21576023), the major accident prevention key projects of State Administration of Work Safety (No. Beijing-0003-2015AQ), and the Fundamental Research Funds for the Central Universities (No. FRF-UM-15-076), and the National Key Research Program of China (2016YFC0700600 and 2016YFC0700603). The cooperation between China and Austria was funded by the Eurasia-Pacific Uninet (No. 18/2014).

Reference

Capelli, L., Sironi, S., Del Rosso, R., Céntola, P., Il Grande, M., 2008. A comparative and critical evaluation of odour assessment methods on a landfill site. Atmos. Environ. 42, 7050-7058.

Capelli, L., Sironi, S., Del Rosso, R., Guillot, J.-M., 2013. Measuring odours in the environment vs. dispersion modelling: a review. Atmos. Environ. 79, 731-743.

Dincer, F., Muezzinoglu, A., 2007. Odor determination at wastewater collection systems: Olfactometry versus H2S analyses. Clean - Soil, Air, Water 35, 565-570.

Gostelow, P., Parsons, S.A., 2000. Sewage treatment works odour measurement. Water Science and Technology. Int Water Assoc, London, UK, pp. 33-40.

Gostelow, P., Parsons, S.A., Stuetz, R.M., 2001. Odour measurements for sewage treatment works. Water Research 35, 579-597.

Guo, H., Jacobson, L.D., Schmidt, D.R., Nicolai, R.E., 2001. Calibrating INPUFF-2 model by resident-panelists for long-distance odor dispersion from animal production sites. Applied Engineering in Agriculture 17, 859-868.

Guo, H., Yu, Z., Lague, C., 2006. Livestock odour dispersion modeling: A review. CSBE/SCGAB 2006 Annual Conference 2006. Canadian Society for Bioengineering, Edmonton, Alberta, p. 170.

Kim, K.-H., Kim, Y.-H., 2014a. Composition of key offensive odorants released from fresh food materials. Atmos. Environ. 89, 443-452.

Kim, K.H., 2010. Experimental demonstration of masking phenomena between competing odorants via an air dilution sensory test. Sensors 10, 7287-7302.

Kim, K.H., 2011. The averaging effect of odorant mixing as determined by air dilution sensory tests: A case study on reduced sulfur compounds. Sensors 11, 1405-1417.

Kim, K.H., Kim, Y.H., 2014b. Composition of key offensive odorants released from fresh food materials. Atmos Environ 89, 443-452.

Kim, K.H., Park, S.Y., 2008. A comparative analysis of malodor samples between direct (olfactometry) and indirect (instrumental) methods. Atmos. Environ. 42, 5061-5070.

Parker, D.B., Koziel, J.A., Cai, L., Jacobson, L.D., Akdeniz, N., Bereznicki, S.D., Lim, T.T., Caraway, E.A., Zhang, S., Hoff, S.J., Heber, A.J., Heathcote, K.Y., Hetchler, B.P., 2012. Odor and odorous chemical emissions from animal buildings: Part 6. odor activity value. Transactions of the ASABE 55, 2357-2368.

Schauberger, G., Piringer, M., Baumann-Stanzer, K., Knauder, W., Petz, E., 2013. Use of a Monte Carlo technique to complete a fragmented set of H2S emission rates from a wastewater treatment plant. Journal of Hazardous Materials 263, 694-701.

Schauberger, G., Piringer, M., Knauder, W., Petz, E., 2008. Re-calculation of the odour emission of a thermal treatment plant for waste by using a Monte-Carlo based model. International Conference on Environmental Odour Monitoring and Control. NOSE 2008, Rome, Italy.

Schauberger, G., Piringer, M., Knauder, W., Petz, E., 2011. Odour emissions from a waste treatment plant using an inverse dispersion technique. Atmospheric Environment 45, 1639-1647.

Thomas-Danguin, T., Sinding, C., Romagny, S., El Mountassir, F., Atanasova, B., Le Berre, E., Le Bon, A.-M., Coureaud, G., 2014. The perception of odor objects in everyday life: a review on the processing of odor mixtures. Frontiers in Psychology 5, 504.

Wenjing, L., Zhenhan, D., Dong, L., Jimenez, L.M.C., Yanjun, L., Hanwen, G., Hongtao, W., 2015. Characterization of odor emission on the working face of landfill and establishing of odorous compounds index. Waste Management.

Wu, C., Liu, J., Zhao, P., Piringer, M., Schauberger, G., 2016. Conversion of the chemical concentration of odorous mixtures into odour concentration and odour intensity: A comparison of methods. Atmospheric Environment, 127, 283-292.