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Conversion of the chemical concentration of odorous mixtures into odour concentration and odour intensity: A comparison of methods

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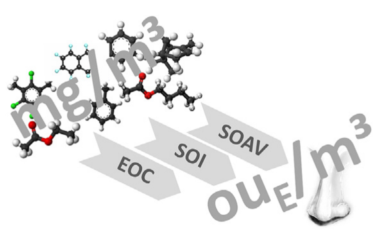
HIGHLIGHTS

- Concentration of odorous substances as surrogate for odour concentration/intensity.
- Comparison of conversion methods with various degrees of complexity.
- Model evaluation by seven VOCs: 23 binary mixtures and 5 mixtures of 7 substances.
- Model input: odour threshold concentration and the slope of the Weber–Fechner law.
- No further calibration by olfactometric measurements necessary.

GRAPHICAL ABSTRACT



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ABSTRACT

Continuous odour measurements both of emissions as well as ambient concentrations are seldom realised, mainly because of their high costs. They are therefore often substituted by concentration measurements of odorous substances. Then a conversion of the chemical concentrations C (mg m^{-3}) into odour concentrations C_{OD} (ou$_E$ m^{-3}) and odour intensities OI is necessary. Four methods to convert the concentrations of single substances to the odour concentrations and odour intensities of an odorous mixture are investigated: (1) direct use of measured concentrations, (2) the sum of the odour activity value *SOAV*, (3) the sum of the odour intensities *SOI*, and (4) the equivalent odour concentration *EOC*, as a new method. The methods are evaluated 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 methods use not only the odour threshold concentration but also the slope of the Weber–Fechner law to include the sensitivity of the odour perception of the individual substances. They fulfil the criteria of an objective conversion without the need of a further calibration by additional olfactometric measurements.

1. Introduction

In the field of environmental odour, it is difficult to realise continuous odour measurements of emission as well as ambient concentrations in the vicinity of an odour source. In many cases,

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odour measurements are substituted by concentration measurements of odorous substances. This indirect method has several reasons. (1) olfactometric measurements need air sampling and several panellists for the measurement, therefore the costs are high, (2) the measurements can only be done discontinuously, and usually inside an odourless laboratory, and (3) in many cases only the emission concentration can be measured, because ambient odour concentrations are often too low to get reliable results (Gostelow et al., 2003).

Continuous odour measurements would, however, be desirable as they can be seen as a prerequisite for several applications. Emission concentration measurements would be required for dispersion modelling to assess the ambient concentration and the related odour annoyance. Measurements of the ambient concentration of odorous substances could be used by environmental protection agencies to monitor the odour annoyance caused by a plant at a certain site (e.g. Kabir and Kim (2010), Schauberger et al. (2011)), and from ambient concentrations of odorous substances, the emission flow rate could be back-calculated by inverse modelling (e.g. Schauberger et al. (2013, 2008)). Moreover, it is agreed that the use of chemical concentrations instead of odour measurements should be limited to cases where the odour concentration is − for some reason − not directly measurable.

Using concentration measurements of odorous substances instead of olfactometric measurements, a conversion of the chemical concentrations C (mg m^{-3}) into odour concentrations C_{OD} (ou$_E$ m^{-3}) and odour intensities OI is necessary, for which several concepts are in use. 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}. This method works well for single substances (e.g. H_2S (Dincer and Muezzinoglu, 2007; Gostelow et al., 2001)) and for a group of substances with a constant composition. To determine the parameters of a regression between concentration and odour concentration, olfactometric measurements have to be performed.

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 in the odour perception, then the sum of the individual OAV is used. This value is called sum of the odour activity value $SOAV$ (Capelli et al., 2013; Parker et al., 2012).

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). It is predominantly used for air quality assessments in Korea. This concept is based on the idea that the perception of an odorous mixture can be calculated by the sum of the individual odour intensities SOI and the related odour concentrations C_{OD} (Kim, 2010; Kim and Kim, 2014b).

The new concept of the equivalent odour concentration EOC introduced here uses the physiological rule that the perception of odour intensity can be assessed by the sum of the stimuli which can be determined by the odour concentration of the individual substances, taking into account the sensitivity of the perception by the slope of the Weber−Fechner law. The goal of the conversion is an objective method, which can be used without the need of an additional calibration by olfactometric measurements.

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. The comparisons will be undertaken both for the single substances as well as their mixtures.

2. Materials and methods

2.1. Conversion methods

The conversion of the concentration measurements of individual substances C_i to odour concentrations of the mixture C_{OD} and odour intensity OI is done by the four different methods briefly outlined in the introduction; the equations used are summarised in Table 1. Besides the concentration of each substance C_i, which is used by all four methods, the necessary additional input is given.

The first method uses the measured concentrations without any further information to assess the odour concentration according to $C_{OD}^C = k_c \sum C_i / m_{OD,0}$, 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}). The proportionality constant k_c can be determined by olfactometric measurements and a linear regression analysis (e.g. Dincer and Muezzinoglu (2007)). In some cases also non-linear functions are in use to describe the relationship between concentration and odour concentration (e.g. power function for H_2S (Franke et al., 2009; Gostelow et al., 2001)). The OI is calculated from the odour concentration by using the Weber−Fechner law (see in detail Section 2.4) with an assumed slope of $k = 1.0$ which results in $OI^C = \log C_{OD}^C + 0.5$.

The second conversion method uses the odour threshold concentration $C_{OT,i}$ of each odorous substance to calculate the odour activity value OAV_i of a certain chemical substance C_i (mg m^{-3}), calculated by $OAV_i = C_i / m_{OD,i}$, using the specific odour mass $m_{OD,i}$, to get the proper measuring unit of an odour concentration (ou$_E$ m^{-3}). The OAV of the entire mixture $SOAV$ is then calculated by the sum of the individual odour activity values $SOAV = \sum OAV_i$ which correspond to an odour concentration. The odour intensity of this mixture is then calculated by the Weber−Fechner law under the assumption of a unity slope $k = 1$ by $OI^{SOAV} = \log SOAV + 0.5$.

The third method was proposed by Kim and Park (2008) 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. The sum of the odour intensities SOI of the entire mixture is then calculated by $SOI = \sum 10^{OI_i}$. The backward calculation of the odour intensity C_{OD}^{SOI} is done for a selected substance j by the Weber−Fechner law (Kim, 2010).

The conversion method introduced here, called equivalent odour concentration EOC, is based on the odour threshold concentration $C_{OT,i}$ and the slope of the Weber−Fechner law k_i. The equivalent odour concentration EOC_j related to one selected substance j of the mixture can be calculated according to $EOC_j = \sum 10^{\frac{k_i}{k_j} \log C_{OD,i}}$ which corresponds to an odour concentration. The odour intensity of this odorous mixture is then calculated by the Weber−Fechner law with $OI^{EOC_j} = k_j \log EOC_j + 0.5$. 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. The conversion of a binary mixture of two odorous substances is depicted in Fig. 1. The odour concentration of substance i is $C_{OD,i} = 100$ ou$_E$ m^{-3}, for substance j, $C_{OD;j} = 100$ ou$_E$ m^{-3}. The slopes are assumed with $k_i = 1.2$ and $k_j = 0.8$, respectively. The conversion of the odour concentration of substance i to the reference substance j with the smaller slope is shown by grey arrows. The equivalent odour concentration related to the reference substance j will result in $EOC_j = 100$ ou$_E$ m^{-3} + 1000 ou$_E$ m^{-3} = 1100 ou$_E$ m^{-3}.

2.2. Chemical substances

Odour concentration measurements of seven chemical substances often emitted by the petrochemical industry were available