COMBINED USE OF AN INVERSE DISPERSION TECHNIQUE AND A MONTE-CARLO MODEL TO COMPLETE THE H$_2$S EMISSION FLOW RATES OF A WASTEWATER TREATMENT PLANT

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Abstract: The assessment of the impact of ambient concentrations in the vicinity of a plant can only be done if the emission rate is known. Based on the measurements of ambient concentrations of H$_2$S and meteorological parameters, the a priori unknown emission rates of a wastewater treatment plant of a tannery are calculated by inverse dispersion modelling. The calculations are done by the Gaussian Austrian regulatory dispersion model. Following this method, the emission data are available however only for the wind directions for which the measuring station is leeward of the plant. Using a Monte-Carlo model, the dataset can be completed also for wind directions for which no ambient concentration measurements are available. First, in a statistical analysis, the cumulative distribution function and the intermittence factor are used to describe the emission scenario. Due to the stochastic character of the emissions, a model is then developed, which is based on the Monte-Carlo technique, to generate a complete data set of the emission rate. For the model validation, the measured ambient concentrations are compared with the calculated concentrations resulting from the synthetic emission data. The cumulative distribution of this new dataset is in good agreement with the empirical data. This Monte-Carlo based technique is a useful supplement for emission rates which are calculated by inverse dispersion modelling.

Key words: Monte Carlo method, inverse dispersion technique, Gauss model, waste water treatment plant

INTRODUCTION

The availability of reliable emission data is the crucial point to apply dispersion models.

The characterisation of a waste water treatment plant WWTP with unknown emissions is derived by using long term measurements of the ambient H$_2$S concentrations leeward of the prevailing wind direction. Based on these measurements and the meteorological data, the emission is re-calculated by an inverse dispersion model. Using this method, the calculation of the emission is possible only in cases when the measuring site is leeward of the pollution source. This means that in the majority of the time no emission data are available. There are many other reasons why emission data can be incomplete (e.g. only short measuring campaigns can be financed, failure of the measuring device, changes in the process flow).

In this paper we present a method which is developed to assess the odour emission of a WWTP over the entire year to calculate H$_2$S exposure in the vicinity of the pollution source.

The model is based on the Monte-Carlo technique that involves using random numbers and probabilities to solve such a problem. This method is often used when the model is complex, nonlinear, or involves more than just a couple of uncertain parameters.

MATERIAL AND METHODS

Inverse dispersion technique

The methodology is described in detail by Schauberger et al. (2011) and therefore repeated here only briefly for clarity. The re-calculation of the emission rate is done with the Austrian regulatory dispersion model (ÖNorm M 9440 (1996); Kolb (1981)). The regulatory model is a Gaussian plume model applied for single stack emissions and distances up to 15 km. Plume rise formulae used in the model are a combination of formulae suggested by Carson and Moses (1969) and Briggs (1975). The model uses a traditional discrete stability classification scheme with dispersion parameters developed by Reuter (1970). Meteorological input parameters to the model are half-hourly values of the wind direction, the wind velocity, and the stability class.

Monte-Carlo model

Due to the statistical structure of the emission flow we use a two-step Monte-Carlo model. For each half hour value two evenly distributed random numbers RN_1 and RN_2 are used. The first stochastic process, using the first random number RN_1, decides on the intermittence factor which describes if an emission value is generated or if the emission value is set to zero.

The second stochastic process, using the second random number RN_2, will generate a value according to the selected cumulative frequency distribution. The evenly distributed random number RN_2 is inverted to a random number, distributed according to an arbitrary distribution function. If $F(x)$ is a distribution function of a random variable x and p is the probability of the realisation in the interval [0; 1], then the quantile function F^{-1}, as an inverse function of the distribution function F, is defined as

$$F^{-1}(p) = \inf\left\{x \in \square \;\middle|\; F(x) \le p\right\}$$

If RN is an evenly distributed random number in the interval [0;1]

$$RN \;\square\; E \quad \text{then} \quad x = F^{-1}(RN)$$

is a random variable, distributed according to the selected distribution function F. As an example, the random number $RN = 0.60$, for a normal distribution $F = \mathbf{N}(\mu, \sigma)$ with the two parameters expected value (arithmetic mean value) $\mu = 2$ and standard deviation $\sigma = 2$, the p-quantile ($p = RN$) with the quantile function gives $F^{-1}(RN) = 2.506$.

Waste water treatment plant and H₂S measurements
The H₂S source is a waste water treatment plant (WWTP) of a tannery. The tannery is situated in Neumarkt (13°44´E, 48°16´N, 390 m a.s.l.) in Upper Austria, a site representative of the Austrian northern pre-Alpine foreland. The surrounding area is rather flat and consists mainly of farmland.

The measuring site was situated in the East of the pollution source, in a distance of about 200 m. The measurements were done by the Environmental Protection Agency of the provincial government of Upper Austria. The H₂S concentration was measured at a height of 3 m above the ground. The level of detection LOD was $C_{LOD} = 0.001$ mg/m³. The measurements of the H₂S ambient concentration and the meteorological parameters were done for a period of about 1½ years (between May 15, 1990 and Dec. 27, 1991).

RESULTS
For the calculation of the emission rate E_{inv} from the inverse dispersion technique, the wind direction is limited to a 30° sector between 255° and 285°. By this selection, the centreline of the plume is close to the measurement site and therefore the lateral distance is limited. The relative frequency for wind directions from this sector is 31%. Excluding small wind speeds below 1.5 m/s which would increase the uncertainty of the calculation of E_{inv} (Flesch et al., 2005; Flesch et al., 2007), the data set is reduced by a further 59 % to ca. 13 % of the entire time series. Only for these remaining data, the emission flow rate E_{inv} can be calculated.

The intermittence factor IF, describing the fraction of non-zero values of the emission rate E_{inv}, is determined to $IF = 0.70$ for the selected wind sector between 255° and 285°.

The cumulative distribution of E_{inv} is depicted in Fig. 1. Due to the limit of detection $C_{LOD} = 1$ µg/m³ and the resolution of the ambient concentration measurements of 1 µg/m³, the cumulative distribution shows a step-by-step increase.

The dataset for the synthetic emission flow rate E_{syn} created by the Monte Carlo model is used to calculate the synthetic ambient concentration C_{syn} for the measuring site, where the ambient concentration C_{meas} was measured. These two data sets of the ambient concentrations are compared to investigate the performance of this two-step method.

The percentiles of the synthetic ambient concentration C_{syn} can be fitted to a log-normal distribution in the same way as the measured data. For the comparison of the measured and the synthetic data we use the same concentration of $C = 1$µg/m³ as a lower limit to truncate the synthetic data in the same way as this was the case for the measurements by the LOD (see also O'Shaughnessy and Altmaier (2011)).

The fitted mean value and the standard deviation of the logarithmically transformed values are determined with $\bar{C}_{syns} = -2.811 \pm 0.009$ (1545 ng/m³) and $\sigma_{syns} = 0.6431 \pm 0.015$ (F-value = 3730, $p < 0.001$, standard error $SE = 0.0121$, and adjusted coefficient of determination $r^2 = 0.9831$). The CDF of the synthetic data shows a shift to higher concentrations and nearly the same standard deviation. To calibrate the synthetic data with the measured

values, we calculate a calibrated data set by $CC_{syn} = \bar{C}_{syn} f_{MV} - \left(C_{syn} - \bar{C}_{syn}\right) f_{SD}$ with the calibrated synthetic ambient concentration C_{syn}, the mean value $\bar{C}_{syns} = -2.811$ and the two calibration factors for the mean value f_{MV} and the standard deviation f_{SD}. The two calibration factors are determined by the ratio of the mean values $f_{MV} = \bar{C}_{meas} / \bar{C}_{syns}$ and the ratio of the standard deviation $f_{SD} = \sigma_{meas} / \sigma_{syns}$, which results in $f_{MV} = 1.157$ and $f_{SD} = 0.9431$
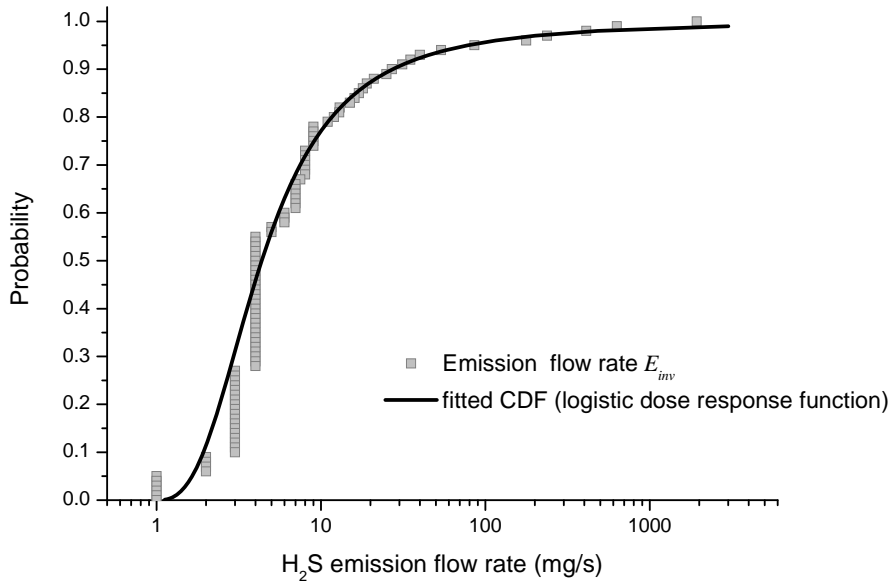

Fig. 1:   Cumulative distribution of the emission flow rate E_{inv}, calculated by the inverse dispersion technique.
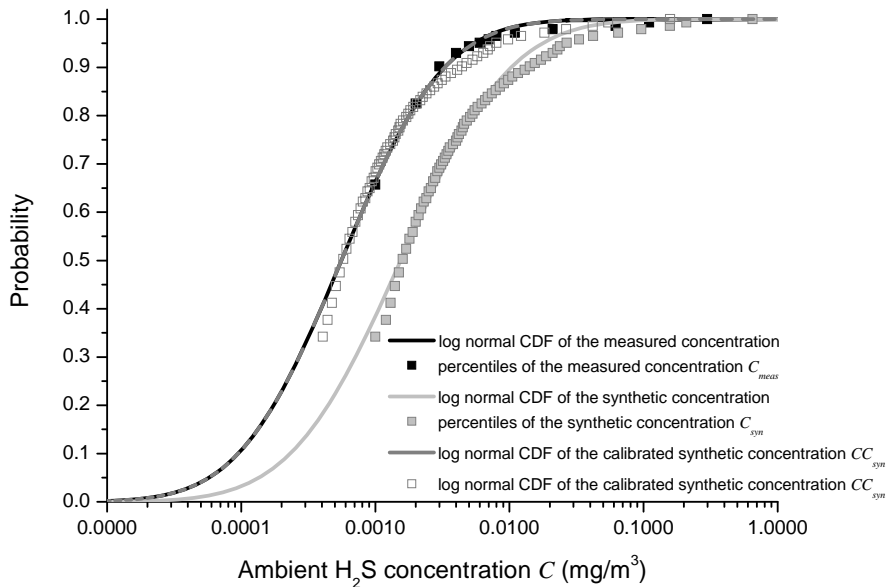

Fig. 2:   Relative frequency (percentiles) and fitted log-normal CDF for the measured ambient concentration C_{meas} (doublets are not shown), the synthetic ambient concentration C_{syn}, and the calibrated ambient concentration CC_{syn}.

The resulting log-normal distribution of the calibrated synthetic ambient concentration CC_{syns} is shown in Fig. 2. The graph for the measured values and the calibrated values cannot be distinguished which demonstrates that the selected approach is successful.

DISCUSSION

There is ample evidence that a one and a half year time series of measured H_2S concentrations in the early Nineties of the last millennium at Neumarkt in Upper Austria was primarily caused by the emissions of a nearby wastewater treatment plant WWTP which today no longer exists. An attempt was undertaken and is described here to re-construct its emissions by a combination of an inverse dispersion technique and a Monte-Carlo based model.

This combined method of the inverse dispersion technique and a Monte-Carlo based technique demonstrates a general methodology to quantify variability of emission rates for a certain plant.

In many cases the pollution source is characterised by a constant value for the emission mass flow. The use of only one (mean) value can lead to an underestimation of the impact of the ambient concentration, calculated by a dispersion model. This error depends on the observed impact of the ambient concentration. In many cases, the health impact is described by a non-linear dose response function (Hilderman and Wilson, 1999). Especially health related phenomena show such a relationship with the ambient concentration C which can be described by a power function C^n with an exponent n in the range between 1.0 and 3.5. Some chemicals show an exponent between 2.0 and 3.0 for the toxicity and fatalities. Only if the exponent $n = 1$, then high concentrations are no longer relevant and therefore the only variable determining toxicity is the mean concentration. However, if $n > 1$, then the use of a constant emission mass flow concentration will underestimate the impact of the substances. The health effects of toxic gases are described in detail by Hilderman (1997).

The Monte-Carlo approach gives the opportunity to calculate a data set of the emission rate for the entire time period with the same statistical features (mean value and standard deviation) as found in the measurements. This means that also for those periods without measured data, the emission rate as input for dispersion models is available. In our case the data gaps are caused by the measurements of the ambient concentration in the leeward of the source. Therefore only one third of half-hour values are available. There are many other reasons why emission data are incomplete if in situ measurements of the emission rate are performed (e.g. only short measuring campaigns can be financed, failure of the measuring device, changes in the process flow, measurements in the lee of the emission source). The method presented allows completing such fragmentary data sets (Schauberger et al., 2013).

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