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Atmospheric tracer experiment uncertainties related to model evaluation

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ABSTRACT

The verification and validation of air quality models is based on comparisons with observational data that can be collected in tracer experiments. The goal of this work is to assess the typical errors that can affect the model evaluation and validation when using real field measurements. The KATREX dataset was chosen for this purpose, since two different teams sampled and analysed concentrations at co-located samplers, therefore providing independent estimates in the same meteorological conditions. Tracers were emitted at two different heights, therefore four datasets are available for the analysis. Comparing the observations of the two teams, also through a statistical analysis, a mean error of 22.5% and a median error of 14% were found. The effect of this uncertainty in the validation of models was then investigated considering the predictions of a Gaussian and a Lagrangian particle models. It followed that the performances of the models could be considered 'good' or not depending on which dataset was used for the evaluation.

1. Introduction

Air quality models are generally evaluated and validated against tracer experiments before being accepted as reliable tools in regulatory applications. In this way it is possible to determine how well they are able to simulate different meteo-diffusion and topographical conditions. Model evaluation is usually performed through a statistical analysis based on the calculations of standard metrics from observed and predicted concentrations at the sampler locations (Chang and Hanna, 2004; Canepa and Irwin, 2005; Bennett et al., 2013). In this kind of analysis the experimental error affecting the observations is therefore implicitly neglected, since its quantification is generally not available to a modeller. In fact, due to the intrinsic non-stationary conditions of the atmosphere, real field experiments can never be reproduced in the same experimental conditions, as opposed to controlled conditions such as wind-tunnel or water channel experiments. Therefore, the estimation of the uncertainties in the observed data is an extremely difficult task. Advanced tools have been developed to evaluate the performances of air quality models (e.g., see Appel et al., 2011; Thunis et al., 2012a). However, while the model simulation uncertainties have been extensively addressed, the problem of estimating the uncertainty in the observations is still open and debated (Jolliff et al., 2009; Dennis et al., 2010; Thunis et al., 2012b). Measurement uncertainty may derive from different errors in the tracer experiment measuring chain: emission, sampling and concentration calculation. Hanna and Paine (1989), examining the Bull Run tracer experiment, noted that "a 6% error in the measured SF6 concentrations translates directly into a 6% discrepancy between observed and predicted concentrations". Thus, it is interesting to investigate which could be the typical uncertainty in real field measurements in order to assess the related error. In this framework, we examined some tracer data from the KATREX data set (Thomas et al., 1983).

The KATREX experiment is suitable for the purpose of this work because of the following features. During one exercise (Schuttelkopf et al., 1981; Thomas et al., 1983), two different teams independently sampled and analysed, with their own devices and for two consecutive 30-min periods, two releases: (1) the same tracer emitted at the 160-m height of the Karlsruhe meteorological tower (Germany); (2) two different tracers simultaneously emitted at the 195-m height of the tower. In particular, at the point at which the maximum ground level concentration (g.l.c.) was expected, each team positioned two samplers. Thus, four estimates, in principle coincident, were done there during the first period. Due to a failure in one of the sampler, only three estimates were available for the second period.

Since the two teams were sampling simultaneously in the same meteorological conditions for both the two periods, the uncertainty

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related to the non-stationarity of the atmosphere is filtered when comparing the two datasets provided by the two teams for the different emissions. Thus, the KATREX experiment allows testing two complementary aspects of the tracer experiments. Firstly, in the 160-m emission case, in which a single gas was emitted, the only possible cause of different g.l.c. estimation is connected to the possible errors in the evaluation chain defined above. In this case, the atmospheric transport and diffusion do not affect the g.l.c. differences among the two team estimations since the meteorological conditions are the same. Secondly, in the 195-m emission case, in which two gases were emitted, there might be two causes for the different g.l.c. estimations: errors in the evaluation chain as in the previous case, and the possible different response of the two gases to the atmospheric transport and diffusion process, if the gases do not behave identically in the atmosphere. The presence of buildings, trees and other obstacles close to the samplers should not interfere with the measurements errors since, in principle, they should affect in the same way the two nearby samplers.

In general, when testing a model against experimental data only one tracer experiment is available, and this is considered as the "truth". Sometimes the concentration standard deviation is available and can be used to estimate the experimental errors. In the KATREX experiment we have instead four different tracer experiments that all claim to be faithful representations of the atmospheric dispersion conditions of that particular time of the day, with its related stability conditions, wind speed and turbulence characteristics. Consequently, through the KATREX experiment it is possible to provide an estimation of the typical uncertainty in a tracer experiment in the real field, and to evaluate how this uncertainty influences the model evaluation, by comparing the g.l.c. observations with model predictions using the four different observation sets.

The outline of the paper is as follows. In the second Section the KATREX experiment and data set is presented. The third Section deals with the comparison of the pairs of concentration estimates generated by the two teams at the various sampler points, in order to assess the average error in the measurements. In the fourth Section we compare the four sets of observed g.l.c. with the prediction of both a simple model, the analytical Gaussian plume model, and of a Lagrangian particle model (Brusasca et al., 1989). The aim of this part of the work is not to assess which of the two models better performs (this was already addressed for the KATREX data set by Brusasca et al., 1989), but to try to understand how the tracer experiment uncertainties influence the performance evaluation of two typical kind of models.

2. The KATREX experiment and the data set

The KATREX data set (Thomas et al., 1983; Thomas and Nester, 1984) collects the results of a series of tracer exercises carried out at the Karlsruhe Nuclear Research Centre (KNRC). This is located near Karlsruhe (Germany) in the Rhine Valley, which is about 40 km wide and is surrounded on both sides by hills as high as 300–400 m. The test field area is flat but rather rough due to the presence of many buildings, some of them belonging to the KNRC (from 10 to 30 m high), forests, rivers, agricultural fields and small villages. Two non-buoyant tracers were always simultaneously released from two platforms of the KNRC meteorological tower (200 m high): Freon-11 ($CFCL_3$) at 160 m and difluorodibromomethane (CF_2Br_2) at 195 m. Comprehensive meteorological information, recorded as 10-min averages, comprises: wind speed and direction at five tower levels (40, 60, 100, 160 and 200 m), the horizontal and vertical wind standard deviations, σ_h and σ_v, at 40, 100 and 160 m, the vertical temperature profile, the net radiation near the ground and the estimated stability class. For all the tracer exercises performed, the KATREX data set also includes the emission data and g.l.c. at various sampling points located on arcs around the tower up to about 8500 m distance (see Fig. 1). In each exercise samples were collected in two subsequent 30 min periods starting about 1 h after the beginning of the emission.

Among the various KATREX exercises we chose the experiment n. 72 because in that case, besides the Karlsruhe team (K_team), a second team (I_team) from Ispra Joint Research Center (IJRC, Italy), took part in the experiment. Both teams simultaneously measured with their own samplers and chemical analysers the tracer ($CFCL_3$) emitted by the K_team at a height H of 160 m (Schuttelkopf et al., 1981; Thomas et al., 1983). Furthermore, the I_team emitted a second tracer (SF_6) from the 195 m platform and sampled and analysed it.

Table 1 illustrates the emission and sampling condition of the selected experiment 72. Ground level samplers were positioned at 5 downwind arcs (approximately at 500 m, 1000 m, 2000 m, 4000 m and 8000 m distance). The samplers of the two teams at the common measuring points were placed at about 2-m distance. The point at which the maximum g.l.c. was expected, and where the two teams positioned two samplers each, is identified hereafter as point n. 24 (see Fig. 1 for its location). Neutral stability conditions prevailed during experiment 72 and the roughness length was estimated by Thomas et al. (1983) to be about 1.5 m.

We mention that the KATREX data set was used by Brusasca et al. (1989) to validate their Lagrangian Particle Diffusion Model LAMBDA against dispersion data observed in the real field. Two experiments were simulated, the exp. 72 as here and exp. 64 that was performed during unstable conditions. These two experiments were also compared to the simulations of ten Gaussian models, differing for the choice of the plume-concentration standard deviations (σ_y and σ_z) and for the way to input the wind speed and direction (either at the emission height or averaged from 40 m to 200 m). In Section 4.2 we will make use of the g.l.c. values produced by LAMBDA that are available on that paper. A rough estimate of the relative error, limited to the point n. 24 and for the 160 m emission only, defined as $C_{max} - C_{min}/2C_{mean}$, where C_{mean}, C_{max} and C_{min} are the mean, maximum and minimum concentrations, resulted to be about 18% and 22% for the first and second period, respectively.

Table 2 reports the meteorological observations during exp. 72. The variables, available at each 10 min, were averaged over 30 min to comply with the concentration sampling time.

To illustrate the turbulence conditions prevailing during exp. 72, Table 2 also includes the horizontal and vertical wind standard

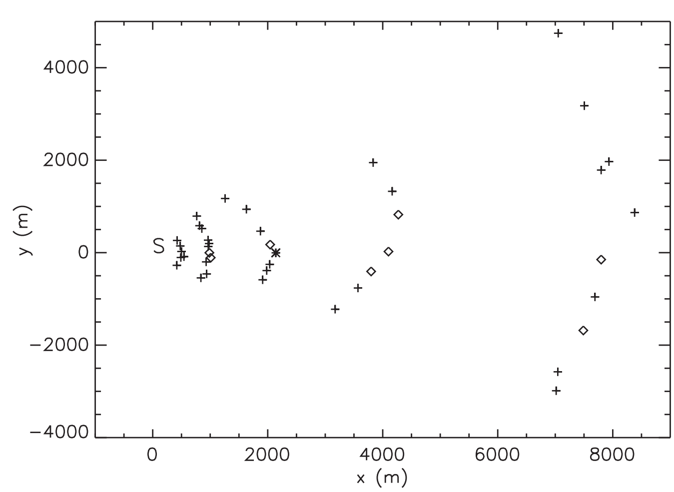

Fig. 1. Locations of the samplers in the experimental domain: diamonds correspond to samplers where simultaneous measurements were collected by the K_team and I_team; the asterisk identifies the location (n. 24) where four samplers were placed and the letter "S" indicates the source position.