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Model quality objectives based on measurement uncertainty. Part I: Ozone

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HIGHLIGHTS

- Proposed performance criteria to evaluate air quality models for O_3 based on measurement uncertainty.
- Derivation of a simplified formulation for O_3 uncertainty based on GUM budgets.
- Performance criteria are station specific and depend on pollutant and concentrations level.
- Performance criteria can be used to set minimum level of quality expected for a given model application.

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ABSTRACT

Since models are increasingly used for policy support their evaluation is becoming an important issue. One of the possible evaluations is to compare model results to measurements. Statistical performance indicators then provide insight on model performance but do not tell whether model results have reached a sufficient level of quality for a given application. In a previous work Thunis et al. (2012, referred to as T2012) proposed a Model Quality Objective (MQO) based on the root mean square error between measured and modeled concentrations divided by the measurement uncertainty. In T2012 the measurement uncertainty was assumed to remain constant regardless of the concentration level. In the current work this assumption is overcome by quantifying all possible sources of uncertainty for the particular case of O_3. Based on these uncertainty source quantifications, a simple relationship is proposed to formulate the measurement uncertainty which is then used to update the MQO and Model Performance Criteria (MPC) proposed in T2012 with more accurate values. The MQO and MPC calculated based on the European monitoring network AIRBASE data provide insight on the expected model results quality for a given application, depending on the geographical area and station type. These station specific MQOs and MPCs have the main advantage of relating expected model performances to the underlying measurement uncertainties.

1. Introduction

Air quality models are powerful tools for the assessment and forecast of pollutant concentrations in the atmosphere. As models are increasingly used for policy support their evaluation is becoming an important issue which is addressed in several documents published by policy-making authorities (EPA, 2009; Derwent et al., 2010; Denby, 2010; ASTM standard D6589, 2005). Models applied for regulatory air quality assessment are commonly evaluated on the basis of comparisons against measurements. This element of the model evaluation process is also known as statistical performance analysis, since statistical indicators are used to determine the capability of an air quality model to reproduce measured concentrations. But although statistical performance indicators provide insight on model performance in general they do not tell whether model results have reached a sufficient level of quality for a given application, e.g. for policy support. In a previous work Thunis et al. (2012, referred to as T2012 in this document) proposed to use as model quality objective (MQO) an indicator based on the root mean square error (RMSE) between measured and modeled concentrations divided by the measurement uncertainty.

Of course the key input to this proposed MQO is the measurement uncertainty. In T2012 the Authors used the Data Quality Objectives (DQO) consisting in the maximum allowed relative uncertainty defined in the EU Air Quality Directive (AQD, 2008). Although DQOs are pollutant dependent, they only apply in the

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region of the Target or Limit Value (LV) set for the considered pollutant. This assumption was therefore considered as a starting point in T2012 which needed to be revised in order to assign more precise performance criteria and MQO in the future.

The goal of this work is to propose more realistic uncertainty estimates that account for dependencies on pollutant concentration. Although sophisticated estimation techniques are applied the final proposed method is kept simple making possible its application by non-experts in metrology. This uncertainty formulation is then used to update the performance criteria proposed in T2012. This paper focuses on O_3 while a companion paper (Pernigotti et al., 2013) extends this approach to NO_2 and PM_{10}.

2. A simplified formulation for the measurement uncertainty

The MQO is built on the conditions that (1) the model and the measurement confidence interval do overlap between each other and (2) the model uncertainty should not exceed the measurement uncertainty (see T2012 for more details). With these two conditions the MQO is defined as the ratio between the RMSE between measured and modeled concentrations and twice the root mean square of the measured expanded uncertainty ($\mathrm{RMS_U}$), as follows:

$$\mathrm{MQO} = \frac{1}{2}\frac{\mathrm{RMSE}}{\mathrm{RMS_U}} = \frac{1}{2}\frac{\sqrt{\sum_{i=1}^{N}(m_i - x_i)^2}}{\sqrt{\sum_{i=1}^{N}U^2(x_i)}} \le 1 \tag{1}$$

Where $U(x_i)$ is the expanded uncertainty of the individual measurement x_i. For condition (1) to be fulfilled, a model results (m_i) should then belong to the interval $x_i \pm 2U(x_i)$. As discussed in T2012, values of this MQO between 0 and 0.5 indicate that, in average, differences between model results and measurement are within the range of their associated uncertainties. Conversely values larger than 1 indicate statistically significant differences between model and measured values. As formulated in (1) the MQO cannot be used straightforwardly as precise values for the measurement uncertainties which depend on the concentration levels are unknown. A simplified relation relating measurement uncertainty to known quantities (e.g. measured mean, standard deviation…) is therefore developed in the following sections.

In recent years, the Guide for the Expression of Measurement Uncertainty (GUM in JCGM (2008)) has been implemented for establishing exhaustive uncertainty budgets for air pollutants (Gerboles et al., 2003; Zucco et al., 2003; Buonanno et al., 2011; Miñarro and Ferradás, 2012; Miñarro et al., 2011). However, GUM is a complex and time consuming approach that needs to be performed for each measurement according to its analytical setup and monitoring conditions. For promoting our model evaluation procedure, a simplified method for uncertainty estimation is needed. Given that the final objective is to define a minimum level of performance to be fulfilled by air quality models, the following derivation will focus on estimating a “maximum measurement uncertainty” (defined later in the document) to be used in the formulation of the MQO (Equation (1)).

The following assumptions will serve as basis to the derivation:

1) The time-series considered in these computations are composed of N elements x_i, representing measurements characterized by a reference time unit. In this work an hourly reference frequency is selected for O_3 as available within the European Air quality database (AirBase, 1997).
2) u_r^{RV} represents an estimate of the relative uncertainty around a reference value (RV). This reference value can be fixed arbitrarily but will be set here for convenience to the hourly/8-h Target Values defined in the AQD (2008) (i.e. 120 μg m^{-3} for O_3).
3) The combined uncertainty of each measurement x_i, $u_c(x_i)$ is decomposed into a component $u_p(x_i)$ proportional to the concentration level and a non-proportional component u_{np} as in Equation (2). Grouping the possible uncertainty sources into these two terms facilitates the estimation of $u_c(x_i)$ as compared to the full application of the GUM methodology.

$$u_c^2(x_i) = u_p^2(x_i) + u_{np}^2(x_i) \tag{2}$$

4) The non-proportional contribution to the combined uncertainty u_{np} is by definition independent of the concentration level and can therefore be estimated around the Reference Value and be assumed to remain equal over the whole range of concentrations. The non-proportional component of the uncertainty is therefore defined as a percentage of the reference value as follows:

$$u_{np}^2(x_i) = \alpha\left(u_r^{RV}\cdot \mathrm{RV}\right)^2 \tag{3}$$

where α is the non-proportional fraction (between 0 and 1) of the uncertainty around the reference value.

5) Similarly the proportional component $u_p(x_i)$ is estimated via the relation:

$$u_p^2(x_i) = (1-\alpha)\left(u_r^{RV}\cdot x_i\right)^2 \tag{4}$$

Combination of Equations (2)–(4) leads to the expression of the measurement uncertainty for a single measurement value x_i.

$$u_c^2(x_i) = \left(u_r^{RV}\right)^2\left[\alpha \mathrm{RV}^2 + (1-\alpha)x_i^2\right] \tag{5}$$

6) Once the combined uncertainty, $u_c(x_i)$ is estimated, the expanded uncertainty, $U(x_i)$ is computed by multiplying $u_c(x_i)$ by a coverage factor, k. Each value of k gives a particular confidence level that the true value lays within the interval of confidence consisting in $x_i \pm U(x_i)$. Most commonly, the expanded uncertainty is scaled by using the coverage factor $k = 2$, to give a level of confidence of approximately 95%. Julious (2004) demonstrated that if two variables, i.e. x_i and m_i, are both characterized by a confidence interval of 95% then the interval built on the condition that these two intervals do overlap (see T2012 for more details) has an associated confidence level of approximately 99%. If x_i and m_i intervals are built with confidence levels of 85% (corresponding to values of k around 1.4) then the overlapping interval would have a 95% confidence level. The coverage factor can therefore be used to adjust the level of stringency of the MQO.

$$U(x_i) = k u_c(x_i) \tag{6}$$

Equations (5) and (6) can finally be combined to obtain an expression for the root mean square of the uncertainty ($\mathrm{RMS_U}$) which can be used in the MQO Equation (1) as follows:

$$\mathrm{RMS_U} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}U^2(x_i)} = k u_r^{RV}\sqrt{(1-\alpha)\left(x_m^2+\sigma^2\right)+\alpha \mathrm{RV}^2} \tag{7}$$