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Indicators to support the dynamic evaluation of air quality models

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HIGHLIGHTS

- Proposed indicators to evaluate air quality models for dynamic evaluation.
- Proposed diagram to evaluate emission reduction impacts on concentrations.
- Assessment of the robustness and non-linearity of model responses.
- Diagram and indicators are useful for policy-maker and model developers.

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ABSTRACT

Air quality models are useful tools for the assessment and forecast of pollutant concentrations in the atmosphere. Most of the evaluation process relies on the "operational phase" or in other words the comparison of model results with available measurements which provides insight on the model capability to reproduce measured concentrations for a given application. But one of the key advantages of air quality models lies in their ability to assess the impact of precursor emission reductions on air quality levels. Models are then used in a dynamic mode (i.e. response to a change in a given model input data) for which evaluation of the model performances becomes a challenge.

The objective of this work is to propose common indicators and diagrams to facilitate the understanding of model responses to emission changes when models are to be used for policy support. These indicators are shown to be useful to retrieve information on the magnitude of the locally produced impacts of emission reductions on concentrations with respect to the "external to the domain" contribution but also to identify, distinguish and quantify impacts arising from different factors (different precursors). In addition information about the robustness of the model results is provided. As such these indicators might reveal useful as first screening methodology to identify the feasibility of a given action as well as to prioritize the factors on which to act for an increased efficiency.

Finally all indicators are made dimensionless to facilitate the comparison of results obtained with different models, different resolutions, or on different geographical areas.

1. Introduction

Air quality models are useful tools for the assessment and forecast of pollutant concentrations in the atmosphere. With their increased use to support policy their evaluation becomes an important issue which is addressed in several documents published by policy-making authorities (EPA, 2007, 2009; Derwent et al., 2010; EEA, 2011; ASTM standard D6589, 2000). Most of the evaluation process relies on the "operational phase" or in other words the comparison of model results with available measurements which provides insight on the model capability to reproduce measured concentrations for a given application. Several statistical performance indicators (e.g. bias, correlation…) and diagrams (Jolliff et al., 2009; Taylor, 2001; Thunis et al., 2012, 2013) have been proposed to support the air quality modelers in this task.

But one of the key advantages of air quality models lies in their ability to assess the impact of precursor emission reductions on air quality levels. Models can then be used to support the design and the assessment of air quality plans by providing insight on the expected impacts of emission abatement measures on concentration levels (e.g. EMEP). Models are then used in a dynamic mode (i.e. response to a change in a given model input data) for which evaluation of the model performances becomes a challenge. This type of evaluation is one of the four steps (operational, diagnostic,

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dynamic and probabilistic) included in the framework for evaluating regional scale numerical photochemical modeling systems proposed by Dennis et al. (2010). So far dynamic evaluation has not received as much attention as its operational counterpart despite the fact that air quality models are regularly applied in this mode for policy support. One of the reason is obviously the greater difficulty to perform this type of evaluation caused by the lack or incompleteness of measurement data.

The Forum for air quality modeling in Europe (Fairmode) guidance document (EEA, 2011) provides some methodological suggestions to perform dynamic evaluation: (1) assess the ability of the air quality model to reproduce historical pollution trends. This exercise brings valuable information on the model capability to react properly to emission changes but it often requires an intensive preparation work in terms of input data (e.g. preparation of past years emission inventories and consistent measurements) and has the drawback of mixing various factors in the analysis (e.g. both emissions and meteorology would change across the years investigated in the retrospective analysis). Examples of applications of this first methodology can be found in Napelenok et al. (2011), Gilliland et al. (2008), Godowitch et al. (2010) or Zhou et al. (2013); (2) assess the model ability to capture the main time variations within the simulated period (e.g. weekly, day–night and/or seasonal). By grouping all data into clusters (e.g. all week-end days within a year) meteorological conditions are mostly filtered out and the impact of emission changes can be more easily identified (Pierce et al., 2010). This methodology can be very useful to identify potential problems in the input data (e.g. emissions time profiles).

These two methodologies still rely on the availability of measurement data to test the dynamic response of the air quality models. One of the obvious methods to further pursue this dynamic evaluation process is to perform model inter-comparison exercises (referred to as probabilistic evaluation). Although no observation are available and therefore no comparison with the "truth" can be made this type of exercise proves to be extremely useful to flag out "strange" model behaviors but also to better understand the model behavior in general (e.g. Eurodelta (Thunis et al., 2010), Citydelta (Cuvelier et al., 2007; Thunis et al., 2007), AQMEII (Solazzo et al., 2012)).

In this work we propose a methodology to support this probabilistic evaluation process but specifically focusing on the dynamic aspects. Similarly to the approach presented in Thunis et al. (2012) for the operational evaluation of air quality models simple indicators and diagrams are developed to support the dynamic evaluation process. These indicators and diagrams aim at synthesizing in systematically information on key aspects of the model responses to emission changes that can be used for policy support.

The indicators proposed in this work aim at responding to the following three questions: (1) what is the impact of given emission precursor reductions in a given geographical area in quantitative terms (or in other words how much of the observed pollution levels originates from the domain of interest and how much from outside?), (2) what is the relative potency (ratio of the abated concentration and abated emissions) of a given precursor with respect to the others and (3) how robust are model responses to emission changes? These indicators are made dimensionless to facilitate their use across regions, models and allow meaningful inter-comparisons.

One of the main objectives of this work is to propose common indicators and diagrams to facilitate the understanding of model responses to emission changes when models are to be used for policy support.

The first section presents the concept and in particular the potencies which are the key element on which the indicators are constructed. In the second section the dynamic indicators are derived and detailed together with a summarizing diagram. The main advantages of these indicators and diagrams are then presented and the information which can be retrieved from them is discussed and examples shown.

2. Definition and concept

In this section the definitions and concepts required to construct the dynamic indicators and associated diagram are presented. These are based on the potency concept, i.e. a measure of the concentration change resulting from an emission reduction. We start with a simple situation in which the pollutant of interest depends only on a single emission precursor and then generalize this to the case in which many precursors have an impact on the pollutant concentration. In both cases a specific section is devoted to the separation of the linear and non-linear impacts since it is a key objective of this work to assess the degree of non-linearity and the robustness of the model responses to emission changes.

2.1. Potency for a single precursor

The **instantaneous potency** for a single pollutant l and precursor k, is defined as the local sensitivity (Yang et al., 1997) of the pollutant l to the emission of the precursor k, i.e. it is the infinitesimal concentration change at a specific location (for example a model grid-cell) resulting from an infinitesimal emission change of a precursor k over a given area A, or in mathematical terms:

$$\dot{P}^k = \frac{\mathrm{d}C}{\mathrm{d}E^k}$$

where
$\dot{P}^k = \dot{P}^{l,k}(x, y; A)$ is the instantaneous potency of pollutant l at the specific location (x, y) affected by the reduction of the precursor k emissions over the area A,

$C = C^l(x,y)$ is the concentration of pollutant l in grid-cell (x,y)
$E^k = E^k(A)$ are the precursor k emissions over the area A.

A finite emission change over the area A can be defined by using a reduction ratio α, as:

$$E^k - E^k_\alpha = \Delta E^k_\alpha = \alpha E^k$$

where $E^k_\alpha = E^k_\alpha(A)$ are the precursor k emissions over area A remaining after the emission reduction α

and $\Delta E^k_\alpha = \Delta E^k_\alpha(A)$ is the precursor k emission change over the area A.

For a finite emission change characterized by a ratio α we define an **average potency** (named potency in the following) as follows:

$$P^k_\alpha = \frac{\Delta C^k_\alpha}{\Delta E^k_\alpha} = \frac{\Delta C^k_\alpha}{\alpha E^k}$$

where $\Delta C^k_\alpha = \Delta C^k_\alpha(x, y) = C - C^k_\alpha$ is the concentration change in which $C^k_\alpha = C^{l,k}_\alpha(x, y)$ is the concentration resulting from the remaining emissions E^k_α

and $P^k_\alpha = \overline{P}^{l,k}_\alpha(x, y; A)$ is the potency.

Note that the same potency value can result from different combination of concentration and emission changes. Indeed a potency of 0.5 can either result from a concentration change of 10