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Application of uncertainty and sensitivity analysis to the air quality SHERPA modelling tool

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ABSTRACT

Air quality has significantly improved in Europe over the past few decades. Nonetheless we still find high concentrations in measurements mainly in specific regions or cities. This dimensional shift, from EU-wide to hot-spot exceedances, calls for a novel approach to regional air quality management (to complement EU-wide existing policies). The SHERPA (Screening for High Emission Reduction Potentials on Air quality) modelling tool was developed in this context. It provides an additional tool to be used in support to regional/local decision makers responsible for the design of air quality plans. It is therefore important to evaluate the quality of the SHERPA model, and its behavior in the face of various kinds of uncertainty. Uncertainty and sensitivity analysis techniques can be used for this purpose. They both reveal the links between assumptions and forecasts, help in-model simplification and may highlight unexpected relationships between inputs and outputs.

Thus, a policy steered SHERPA module - predicting air quality improvement linked to emission reduction scenarios - was evaluated by means of (1) uncertainty analysis (UA) to quantify uncertainty in the model output, and (2) by sensitivity analysis (SA) to identify the most influential input sources of this uncertainty. The results of this study provide relevant information about the key variables driving the SHERPA output uncertainty, and advise policy-makers and modellers where to place their efforts for an improved decision-making process.

1. Introduction

Air quality has significantly improved in Europe over the past few decades (EEA, 2017), but exceedances of the legislative limit values still persist, mainly for pollutants such as ozone (O_3), nitrogen dioxide (NO_2) and particulate matter (PM10 and PM2.5)[1]. While, in the past years, these exceedances were wide-spread across Europe, they now tend to concentrate in specific regions or cities (Kiesewetter et al., 2015). This new and changed situation calls for a novel approach tailored to local air quality management (to complement EU-wide existing policies).

There is a long standing tradition of using modelling techniques in supporting the design of air quality policies. A first set of techniques consists of three dimensional numerical models that simulate transport, chemistry, emissions, and deposition in the atmosphere (Mailler et al., 2016; Pernigotti et al., 2013). Given their complexity and demanding/onerous requirements (in terms of data preparation, scientific/technical knowledge and computing time), these models are mainly used for scientific research. For such models, state-of-the art approaches are available to compute sensitivity coefficients measuring how the concentrations predicted by the model depend on input data and model parameters. These approaches vary from conceptually simple ones, as the brute-force (varying the input parameters one by one in separate model simulations and evaluating the change in predicted concentrations) to more complex, as decoupled direct method and the adjoint method (Dunker et al., 2002; Sandu et al., 2003; Kelly et al., 2015). All these methods are usually applied to a fully-fledged air quality model, to perform its local sensitivity analysis.

In addition to three dimensional numerical models, another set of approaches has been developed, mainly to deal with the 'science-to-policy' interface. These approaches are referred to as "Integrated Assessment Models", as they integrate various dimensions: policy costs, benefits, etc … in one single approach. In such type of approaches, the air quality component is not based on the full air quality model

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[1] PM: inhalable particles, with diameters that are 10 or 2.5 micrometers.

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previously mentioned (that would be too time consuming to be simulated) but usually it is implemented as a "surrogate" of the full air quality model. A valuable example of "Integrated Assessment Model" is the GAINS-EU (Greenhouse Gas - Air Pollution Interactions and Synergies) integrated assessment model (Amann et al., 2011), which is based on linear source-receptor relationships to link emissions to concentrations, and has frequently been used to choose optimal emission reductions per country, in order to achieve environmental improvements at a minimum cost. In the last years, given the current situation marked by regional and/or local (city) hot spots, the EU integrated assessment modelling tools have also been complemented/aided by both regional and local approaches. This has been done in recent years using national versions of GAINS based on finer scale modelling (as in GAINS-Italy, D'Elia et al., 2009), or with regional tools (as RIAT, the Regional Integrated Assessment Tool, Carnevale et al., 2012, Carnevale et al., 2014, Pisoni et al., 2010). These efforts have already supported the implementation of regional/local plans, but it is important to bear in mind that their application heavily relies on the availability of detailed local data and of complex scientific/technical know-how, not always readily available on a local scale.

Recently, the SHERPA (Screening for High Emission Reduction Potentials on Air quality) modelling tool was developed (Clappier et al., 2015; Thunis et al., 2016; Pisoni et al., 2017) to provide an alternative approach. SHERPA, which is based on a "surrogate model" replicating the behavior of a fully-fledged air quality model, serves as a tool to support regional/local decision makers responsible for the design of air quality plans. It is distributed with default data that covers the whole Europe and enables decision-makers to work on their own regional domain. It can be used without the need to perform prior complex scientific/technical tasks. SHERPA supports decision-makers who need to plan air quality policies by implementing modules such as "source allocation" (to apportion air pollution in terms of sectors and precursors of origin), "governance" (to identify the key geographical entities contributing to the pollution in one specific area), "scenario" (to test the effect on air quality of a given sector-specific emission abatement scenario). As the tool will be used in the policy arena, it is of utmost importance to evaluate the robustness of the model predictions with regards to various sources of uncertainty.

Uncertainties can be particularly influential in policy context. It is widely known that model and data are uncertain and that uncertainties may be very significant. It is therefore important to know how model outputs, namely potential policy impacts are affected by these uncertainties. The uncertainty quantification process helps to understand whether models are "fit for the purpose" and/or apt to be used in the field of policy making. Complementary to this, sensitivity analysis (SA) should also be applied. While the uncertainty analysis (UA) aims at quantifying uncertainty in the model output, sensitivity analysis investigates the dependency of the model output from various sources of uncertainty in the model inputs (Saltelli et al., 2008). Sensitivity analysis is an important ingredient in the quality assurance of models used for evidence-based policy and, because it reveals the links between assumptions and predictions, it helps in model simplification (i.e. not relevant input can be identified) and model calibration (i.e. optimal parameters setting). It can highlight unexpected relationships between inputs and outputs, helping to identify regions of the input space which are responsible for critical values of the output.

In this paper, we perform the uncertainty and sensitivity analysis of the SHERPA "scenario" module (Thunis et al., 2016). This module allows for the estimation of how concentrations change due to various given emission-reduction scenarios. It is used as a basis for all SHERPA modules and is therefore the key element to be tested. As SHERPA is a model characterized by spatially-varying coefficients and inputs, the Uncertainty and Sensitivity Analysis (UA-SA) have been performed on a few selected cities (Helsinki, Constanța, London, and Milan, see Fig. 1), representative of different meteorological and of varying emission inventory conditions (the same analysis is presented in Albrecht et al., 2018 on an extended set of cities, showing similar conclusions; so here, for lack of space, we focus on a smaller number of cities). This analysis focuses on two main issues: (1) what is the robustness level of the SHERPA results in terms of uncertainty of the model response (uncertainty analysis) and (2) how the model output is influenced by each model input – parameters, precursors, and policy choices (sensitivity analysis).

In this study we answer these research questions within a Global Sensitivity Analysis (GSA) variance-based framework. As opposed to local sensitivity analysis (i.e. with brute-force, decoupled direct and adjoint methods, previously discussed), GSA measures the relative importance of the model inputs by exploring the entire input space. In particular, GSA has been carried out using the popular methods described in Saltelli et al. (2010). The results provide information about the key variables driving the SHERPA output uncertainty. This paper is organized as follows: In Section 2, we briefly introduce the SHERPA model and the sensitivity analysis method employed to analyze it. In Section 3, we define the model input uncertainties. Furthermore, we discuss the results in Section 4 before reaching our conclusion in Section 5.

2. Materials and methods

In this chapter the SHERPA model (both formalization and its assumptions/caveats) and the technique used to evaluate uncertainty and sensitivity analysis are presented.

2.1. The Sherpa model

SHERPA has been developed to provide a speedy modelling approach to calculate concentration fields resulting from emission reduction scenarios, mimicking the behavior of a full Chemical Transport Model (CTM). CTMs provide pollutant concentration fields that account for the complex transport, diffusion and chemical processes occurring in the atmosphere. The aim of SHERPA is to mimic CTMs' behavior with a simpler relationship/equation derived from a set of full CTM simulations built with various emission reduction scenarios. This set of scenarios should be sufficiently varied (in terms of concentration changes, responses to emission changes) to provide the SHERPA training phase with sufficient data variability.

In SHERPA, concentration changes due to an emission reduction scenario are computed on a cell by cell basis according to the following equation:

$$\Delta C_n = \sum_{p}^{N_{prec}} \sum_{m}^{N_{cell}} a_{n,p,m} \Delta E_{p,m}, \ \forall\, n \in [1, N_{cell}] \tag{1}$$

where the delta concentration ΔC_n (change of concentration in comparison to the base case) in a receptor grid cell "n" is expressed as a linear combination of the emissions delta $\Delta E_{p,m}$ (variation in emission when compared to the base case), for each source cell "m" and pollutant (i.e. precursor) "p". The $a_{n,p,m}$ coefficients act as weighting factors which apportion the amount of emission variation $\Delta E_{p,m}$ of precursor p stemming from cell m and reaching cell n. As the correlation between ΔC_n (at receptor cell n) and $\Delta E_{p,m}$ (at all sources cell m) decreases with the distance between the cells, it has been assumed that the coefficients $a_{n,p,m}$ in the previous equation can be approximated by the following distance-function:

$$a_{n,p,m} = \alpha_{n,p}(1 + d_{n,m})^{-\omega^{n,p}} \tag{2}$$

where $d_{n,m}$ is the distance between cells n and m and the two unknowns α and ω for each precursor p and each grid cell n were estimated from CTM simulation results (see Pisoni et al., 2017 for more details).

Even though the previous equations remain the same/unvaried everywhere in the whole calculation domain, the values of α and ω are grid-cell specific. The parameter α is related to the amplitude of the