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A new approach to design source–receptor relationships for air quality modelling

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ABSTRACT

Air quality models are often used to simulate how emission scenarios influence the concentration of primary as well as secondary pollutants in the atmosphere. In some cases, it is necessary to replace these air quality models with source–receptor relationships, to mimic in a faster way the link between emissions and concentrations. Source–receptor relationships are therefore also used in Integrated Assessment Models, when scenario responses need to be known in very short time. The objective of this work is to present a novel approach to design a source–receptor relationship for air quality modeling. Overall the proposed approach is shown to significantly reduce the number of simulations required for the training step and to bring flexibility in terms of emission source definition. A regional domain application is also presented, to test the performances of the proposed approach.

1. Introduction

Air quality models are complex tools which include detailed representations of the transport, diffusion and chemical processes taking place in the atmosphere. These models work at various horizontal and vertical resolutions and account for the non-linear interactions in each of the processes previously mentioned.

One of the main advantages of AQ models is the possibility to assess the impact of emission changes on concentration levels. The easiest approach is to modify the emissions accordingly, run the model and check the resulting concentrations. This is generally referred to as using a model in "scenario mode". One of the consequences of the high complexity of AQ models is their associated CPU time implying that AQ models can only be run for a limited set of scenarios due to this important constraint. If the number of required scenarios becomes prohibitive, one way out is to design source–receptor relationships (or models), which is a simplified modeling approach that will mimic the full air quality model behavior. Air quality integrated assessment models use this approach when scenario responses need to be known in very short time within an optimization process. In this case a simplified model is constructed to link the emission changes to the concentration changes. The same type of simplified model is also very useful in scenario mode when a user wishes to assess the impact of several possible emission reductions on concentrations without requiring the long computation times that come with running the full AQ model.

Many examples of this approach do exist in literature. Seibert and Frank (2004) developed linear-source receptor relationships to compute the transport of atmospheric traces substances with a Lagrangian particle dispersion model. Simpson et al. (1997) and Tarrason et al. (2004) used the Eulerian EMEP model as basis to compute country-to-country source–receptor relationships over a European domain, considering a multi-annual time-frame. At the national scale, Vedrenne et al. (2014) used a similar approach over Spain with the Atmospheric Evaluation and Research Integrated model for Spain (AERIS). This model allows for assessing the impact of sectorial emission reductions on air quality. All the above mentioned techniques however rely on a large number of computer simulations to identify the source–receptor models.

Alternative approaches also exist to assess the impacts of emission scenarios on air quality. The decoupled-direct method (DDM) (Dunker, 1981, Dunker et al., 2002) or its adjoint sensitivity complementary method (Sandhu et al., 2005; Hakami et al., 2006) provide sensitivity coefficients based on an initial set of nonlinear, partial differential equations. These sensitivity coefficients can then

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be used to describe how emissions impact air pollution concentrations. The source-oriented external mixture (SOEM) method (Ying and Kleeman, 2006) or the Particulate Source Apportionment Technology (PSAT) method (Wagstrom et al., 2008) use a source-oriented Eulerian air quality model and monitor the formation of PM2.5 nitrate, sulfate and ammonium ion from primary particles and precursor gases emitted from different sources. However these techniques usually require an a-priori definition of the sources and receptors to be tracked with a requested computer time quickly increasing with the number of these tracked sources/receptors. In this work we will only focus on the formulation of source–receptor relationships on the basis of an Eulerian air quality model.

Given the scope of the source–receptor (SR) model (e.g. focus on yearly averaged model responses), an experiment is designed and assumptions are made to construct the SR model. This experiment consists in the following steps: (1) running several times the full AQ model under selected conditions (training), (2) designing the SR model to mimic at best the source-receptor relations of the full AQ model and (3) validate the SR model on a series of independent simulations. All three steps need to be designed to make sure the SR model becomes a good representation of the full air quality model for the desired scope and that the assumptions made during the derivation are robust.

The objective of this work is to present a novel approach to design a source–receptor model for air quality modeling. The main advantages of the proposed approach lie in the reduced number of simulations required for the training step as well as in the flexibility it brings in terms of source definition. In a first section, we will introduce the overall problem of source–receptor relationships. We then detail possible approaches to simplify the problem both in terms of sources and receptors. In a second section an application on a regional domain is presented, where different configurations are tested.

2. Methodology

2.1. Setting the "source–receptor" problem

The full AQ model operates for a given time period over a given geographical area. Both the emission input and the concentration output are spatially gridded over this geographical area. Although it is the same grid, we make here a distinction between the source (emissions) and the receptor grids (concentrations) for convenience.

Prior to any assumption being made, each receptor cell relates with every source cells, i.e. each grid cell concentration depends on the emissions coming from every grid within the domain. Moreover, different emission precursors can have an effect on the given concentration, i.e. emissions from each precursor in every cell relates to the concentration observed in a single cell (Fig. 1). This relation between precursor and receptor cells can be formalized mathematically using a relation containing several coefficients. For linear relationships, only one coefficient is required to link one receptor cell to one source cell but the number of coefficients increases with the degree of non-linearity characterizing the relations. The exact number of coefficients will depend on the shape of the non-linear function used (or the sum of non-linear function used). These functions which characterize the S/R relationship are identified by performing different scenario simulations with the full AQ model.

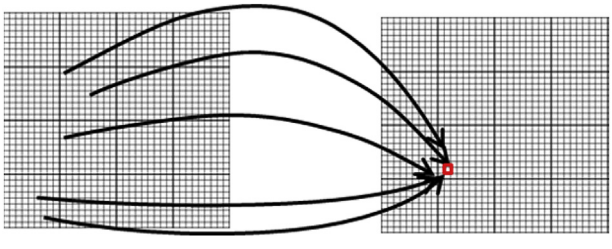

Fig. 1. General configuration of a source–receptor model, separating source (emissions) and receptor (concentrations) grids.

In this work we will focus on particulate matter (PM10) yearly averaged concentrations which are assumed to depend on the following five emission precursors: Nitrogen oxides (NOx), Volatile Organic Compounds (VOC), Sulfur Dioxides (SO2), Primary Particulate Matter (PPM) and Ammonia (NH3). Since Thunis et al. (2015) showed in their application of a full AQ model over three domains in Europe that non-linear effects were marginal and could be neglected for yearly/seasonal averaged PM10 model responses, we will assume linearity in the following derivations and considerations, leading to the following equation for a given receptor cell "j":

$$C_j = C_j^0 + \sum_{p}^{P} \sum_{i}^{N} a_{ij}^{p} E_i^{p} \quad (1)$$

where N is the number of source grid cells within the domain and P is the number of precursors. As seen from this equation, the relation between each precursor (p) in each source cell (i) and a receptor cell (j) is linear, therefore characterized by one constant (a_{ij}^{p}). Although a linear relation needs only one coefficient to be defined the number of unknowns (P × N+1, i.e. the N × P a_{ij}^{p} coefficients plus the background C_j^0) remains important and can easily lead to a non-manageable number of simulations to be performed with a full AQ model (e.g. the number of unknowns would reach 12501 for a domain of 50 × 50 cells and 5 precursors).

The coefficients a_{ij}^{p} in Equation (1) are the absolute potencies described in Thunis and Clappier (2014) defined as the ratio of the concentration change (with respect to the base-case) to the associated emission change, for a given scenario. It is also important to point out that while the approach followed in Equation (1) is precursor driven, the approach could easily be adapted to macro-sectors.

In the next two sub-sections we will analyze how the problem can be simplified by aggregating the source cells and/or receptor cells (i.e. the coefficients a_{ij}^{p} will be assumed to be constant over a range of source and/or receptor cells).

2.2. Fixed source aggregation and 1 cell receptor window

In this configuration, source grids are aggregated in fixed geographical entities, e.g. countries, regions or set of regions/countries while receptor grids are still considered cell per cell (Fig. 2 top, illustrated for two countries). This approach is used in GAINS-EU (Amann et al., 2011), GAINS-IT (Mircea et al., 2014 and D'Elia et al., 2009) or in the TM5-FASST models.

The number of unknowns is then directly proportional to the number of geographical entities selected. Equation (1) then transforms into:

$$C_j = C_j^0 + \sum_{p=1}^{P} \sum_{i=1}^{N_A} a_{ij}^{p} E_i^{p} \quad (2)$$

where N_A is the number of emission aggregation zones selected and E_i^{p} is the precursor "p" emission of the fixed entities "i". In this case the minimum number of required scenarios is equal to the number of unknowns (i.e. P × N_A+1).