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Adding spatial flexibility to source-receptor relationships for air quality modeling

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ABSTRACT

To cope with computing power limitations, air quality models that are used in integrated assessment applications are generally approximated by simpler expressions referred to as "source-receptor relationships (SRR)". In addition to speed, it is desirable for the SRR also to be spatially flexible (application over a wide range of situations) and to require a "light setup" (based on a limited number of full Air Quality Models - AQM simulations). But "speed", "flexibility" and "light setup" do not naturally come together and a good compromise must be ensured that preserves "accuracy", i.e. a good comparability between SRR results and AQM.

In this work we further develop a SRR methodology to better capture spatial flexibility. The updated methodology is based on a cell-to-cell relationship, in which a bell-shape function links emissions to concentrations. Maintaining a cell-to-cell relationship is shown to be the key element needed to ensure spatial flexibility, while at the same time the proposed approach to link emissions and concentrations guarantees a "light set-up" phase. Validation has been repeated on different areas and domain sizes (countries, regions, province throughout Europe) for precursors reduced independently or contemporarily. All runs showed a bias around 10% between the full AQM and the SRR.

This methodology allows assessing the impact on air quality of emission scenarios applied over any given area in Europe (regions, set of regions, countries), provided that a limited number of AQM simulations are performed for training.

1. Introduction

Like in any other policy area, modeling tools are nowadays commonly used in the field of air pollution, to support policy makers in choosing the best options to improve air quality (Reis et al., 2005; Terrenoire et al., 2015). Air quality models (AQM) indeed represent the best (and only) instruments to screen and assess the impact of future policy options. But because these models include the current state of the art in terms of physical and chemical representation of the complex processes taking place in the atmosphere (captured through the numerical resolution of complex nonlinear differential equations) they generally run slow in terms of computer time and do not allow for the interactivity required by policy makers when testing various options in relation to possible air quality plans.

This problem is exacerbated when AQMs are used in the frame of complex integrated assessment modeling (IAM) tools. IAMs have been extensively used in different policy related scales/contexts, as e.g. at the international level in support to preparation of the LRTAP (United Nation Economic Commission for Europe "Air Convention") Gothenburg protocol (Amann et al., 2011), at European level in the frame of the National Emission Ceilings and Air Quality Directive (Kiesewetter et al., 2015), or at the national/local scales to elaborate plans and programs to improve air quality (Carnevale et al., 2014). But due to computing power limitations in IAM applications, AQM are generally approximated by simpler expressions that guarantee speed and interactivity. These expressions, often referred as "source-receptor relationships (SRR)" approximate the behavior of the complex air quality model with the objective of providing simple relationships between emissions and concentrations (Oxley et al., 2007; Pistocchi and Galmarini, 2010; Ratto et al., 2012). The first step to derive SRR consists in running the full AQM with

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different input data (i.e. emissions) that cover the desired range of future application. This step is referred to as training. In contrast, the validation phase consists in running a few AQM simulations to test the capacity of the SRR to mimic the AQM in different applications. For a meaningful evaluation, these simulations should be independent from the training simulations.

In addition to speed, it is desirable that the SRR also fulfill other characteristics, namely "spatial flexibility" and "light set-up". By "spatial flexibility" we intend here the possibility of applying the SRR over a wide range of possible situations, in terms of the spatial design of the scenarios (i.e. having freedom in defining the areas where emission reductions will be applied). By "light set-up" we mean both that the number of full AQM simulations requested for the training of the SRR should be limited, and that the level of knowledge required for the analyst to train the SRR should be limited (i.e., using simple regression techniques, etc …). Given the complexity of the AQM and the time required to perform simulations, it is important to keep the number of simulations in the training set under control, without compromising accuracy. Speed, flexibility and light setup do not naturally come together and a gain in spatial flexibility will most of the time be obtained at the expense of a heavier set-up or of a loss in terms of speed. The challenge therefore consists in ensuring a good compromise among these three characteristics, while preserving accuracy, i.e. a good comparability between SRR results and AQM.

According to their purpose, currently used SRR methodologies generally privilege one or two of the above mentioned characteristics in detriment of the others. The GAINS ("Greenhouse Gas - Air Pollution Interactions and Synergies", Amann et al., 2011, Kiesewetter et al., 2015) integrated assessment tool relies on the EMEP ("European Monitoring and Evaluation Programme") air quality model to build its SRR (Tarrasón et al., 2004). In this approach, emissions are aggregated in terms of countries, resulting in "country-to-grid" SRR. Being proportional to the number of countries and emission precursors considered, the number of simulations requested for the training is substantial. Given the way they are constructed, the country-to-grid EMEP SRR can only be applied to assess the impact of scenarios in which emissions have been changed over the countries considered during the training. This results in a lack of spatial flexibility, i.e. the impossibility to use SRR to evaluate subnational emission reduction scenarios. The GAINS-EMEP SRR, however, run fast as the number of operations is proportional to the number of countries and precursors involved.

In the AERIS ("Atmospheric Evaluation and Research Integrated system for Spain") model emissions are not aggregated spatially but in specific sectors (Vedrenne et al., 2014). Full AQM simulations in which these sectors are reduced individually are then used in the training phase to construct the SRR. Because the number of requested simulations is proportional to the number of sectors considered, the setup can be quite light. Spatial flexibility is on the contrary absent because all emission reductions considered in the training are performed domain wide. Similarly to the EMEP SRR, this approach also runs fast.

Another methodology has been implemented in the RIAT + tool (Carnevale et al., 2012). Emissions are here aggregated in four large quadrants that are defined relatively to each grid cell of the domain (sliding quadrants). The quadrant emission values and their related grid cell concentrations are then used to feed a neural network that delivers the SRR (Carnevale et al., 2009). Although the approach requires a limited number of full AQM simulations (around 20), the set-up of the SRR remains complex due to the need of implementing neural networks. Neural networks also require that their application is limited to the range of situations covered during the training phase. From a speed point of view, the sliding quadrant-to-cell approach performs very well.

Clappier et al. (2015) (referred as C2015 in the following) proposed a new methodology (referred to as "Multi-ring") to derive SRR. Similarly to the quadrant-to-cell approach described above, these SRR make use of sliding emission aggregations (rings) but assume linearity in the emission-concentration relationships. The main consequence of this linearization is the simplification of the training phase.

In this work, we further elaborate on the approach of C2015 and show how it can be further developed to improve spatial flexibility. In Section 2, we briefly review the main elements of the C2015 work and discuss its limitations in terms of spatial flexibility. In Section 3 an improved methodology is proposed while Section 4 evaluates the results of this approach for a series of case-studies.

2. The "multi-ring" approach and its limitations

In this section we briefly review the C2015 methodology main features and limitations.

2.1. Methodology

As previously stated, the goal of the SRR is to mimic an AQM to calculate as quickly as possible the effect of emission reductions on concentration levels (Castelletti et al., 2012). In general, the SRR model consists in an algebraic relationship between gridded emissions and concentrations. Although concentrations and emissions are defined on the same grid cells, we make here a distinction between sources (emissions) and receptors (concentrations) grids for convenience.

A series of steps are detailed in C2015 in order to design the SRR, which are briefly summarized as follows:

1) The calculation of SRR algebraic relationships between emissions and concentrations expressed in absolute terms can lead to errors if not accounted for correctly. This problem disappears if emission and concentration are expressed in relative terms, i.e. as difference (delta) between a base case and a reduction scenario (Thunis et al., 2016).
2) For long term indicators (i.e. yearly average) which are the focus of this work, the relationship between emission and concentration deltas can be approximated accurately with a linear function (Thunis et al., 2015). Consequently and since the concentration change in a receptor cell "*j*" can result from the reduction of different emission precursors "*p*" coming from any source cell "*i*" within the domain, the concentration delta in a receptor cell "*j*" can therefore be computed as follows:

$$\Delta C_j = \sum_{p}^{P} \sum_{i}^{N} a_{ij}^{p} \Delta E_i^p \tag{1}$$

where N is the number of source grid cells within the domain, P is the number of precursors, ΔE_i^p and ΔC_j are the emission and concentration deltas, a_{ij}^p are unknown parameters to be identified.

3) The number of unknown parameters (a_{ij}^p) which need to be identified in the case of a cell per cell relationship is prohibitive (equation (1)). Indeed for a $N = 50 \times 50$ grid cells domain and $P = 5$, the identification of about 12,500 parameters is required to calculate ΔC_j. 12,500 unknown parameters would need to be identified by solving an equations system that contains at least 12,500 equations, each of these relying on ΔC_j and ΔE_i^p provided by an independent CTM scenario run, which is materially unfeasible.