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Why time and space matters - arguments for the improvement of temporal emission profiles for atmospheric dispersion modeling of air pollutant emissions

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Abstract:

Emissions of trace gases originating from anthropogenic activities are vital input data for chemical transport models (CTMs). Other key input datasets such as meteorological drivers, and biogeochemical and physical processes have been subject to detailed investigation and research in the recent past, while the representation of spatio-temporal aspects of emission data in CTMs has been somewhat neglected. Arguably, this has less impact on the regional to hemispheric or global scale, where the grid sizes of currently applied CTMs represent well mixed average concentrations or deposition values. Evaluating model output against ground-based observations or remote sensing results on these spatial levels may not to be overly sensitive to the temporal (and spatial) profiles of emission input data.

With increasing level of detail and spatio-temporal resolution, CTMs applied to determine national or local scale air quality are likely prone to be more sensitive to the spatial and temporal patterns of anthropogenic emissions. The location and timing of emission events - for instance peaks of ammonia emissions following the spring and autumn application of manure and mineral fertilisers - may well determine local concentration or deposition episodes, while not necessarily affecting seasonal or even annual mean values. In a similar way, high levels of ambient ozone concentrations typically have very strong seasonal and diurnal variations, with effects on plants for instance varying greatly over time. In addition to that, the timing of occurrences of high ambient concentrations plays a vital role in the assessment of compliance with air quality limit values.

This paper illustrates the general need for taking into account the spatial and temporal resolution of air pollutant emissions, using some examples of recent work conducted in the UK for national scale atmospheric dispersion modeling.

Keywords: atmospheric dispersion modeling, emissions, temporal resolution, spatial resolution

1. INTRODUCTION

Atmospheric dispersion models are vital tools for the assessment of regional and local air quality and for monitoring compliance with air quality limit values. They are filling the gap that exists because it not feasible to establish continuous and comprehensive real-time monitoring everywhere, for all relevant air pollutants and at all times to quantify potential health effects on humans or impacts on ecosystems based on monitoring data. In many cases, the ex-ante impact assessment of policies is conducted based on model results, as well as the ex-post evaluation of the effectiveness of policies or compliance monitoring regarding the achievement of air quality limit values and other indicators.

As computing power is continuously increasing, atmospheric dispersion models have been substantially pushing the limits of temporal and spatial resolution, covering spatial scales from global and hemispheric down to local level and decades to seconds in temporal terms. However, the main emphasis in model development has been on improving the process-representation within the models to achieve better fits of modeled vs. observed atmospheric conditions and chemical transformation. While this is essential, the spatial and temporal representation of a key input data set - emissions of pollutants and other trace gases - has not been improved in the same way. The spatial resolution of emission data has been subject to some improvements in recent years, with national inventories available for modeling typically providing data on 1×1 km or 5×5 km, on the regional or European scale, the current 50×50 km inventories are due to be generated in 10×10 km resolution. Different projects even provide specific emission maps for selected pollutants or study regions down to 1×1 km (see Fig. 1). In the following, the discussion will thus focus on the temporal resolution, which has not been addressed much if at all.

The spatio-temporally explicit generation of emissions for atmospheric transport and chemical transformation modeling of air pollutants in general has been addressed in the past e.g. in the EUROTRAC subproject GENEMIS (Friedrich and Reis, 2004). Other publications (see Gilliand *et al.*, 2003; Pinder *et al.*, 2004a, b; Gyldenkærne *et al.*, 2005; Hellsten *et al.*, 2008; Reis et al., *in preparation;* Skjøth *et al.*, 2004 & 2010) have addressed specific issues and topics (in this case mainly agricultural ammonia, because of the dual influence of human activities and meteorological parameters), but so far the representation of detailed temporal profiles of (anthropogenic) emissions in models has not been addressed in a comprehensive way. Issues of spatio-temporal scale, however, are not only relevant for atmospheric modelling, but equally in a subsequent stage of the environmental impact assessment process (see for instance Oxley and ApSimon, 2007).

In this paper, we will elaborate on the underlying rationale and need for a general change in paradigm in relation to the spatio-temporal resolution of emission input data for modeling. The work on which this evaluation is based has been conducted in the frame of the EMEP4UK model development, which has been described for instance in Vieno *et al.* (2011), while looking at the wider picture to derive more generally applicable conclusions.

To begin with, we will look at both the main drivers for spatial and temporal variations in emission input data specifically, while taking into account the same variations of other model input and the potential influence on model results. In a second step, the needs and requirements for temporally and spatially accurate representations of model output will be discussed in the context of the science-policy interface.

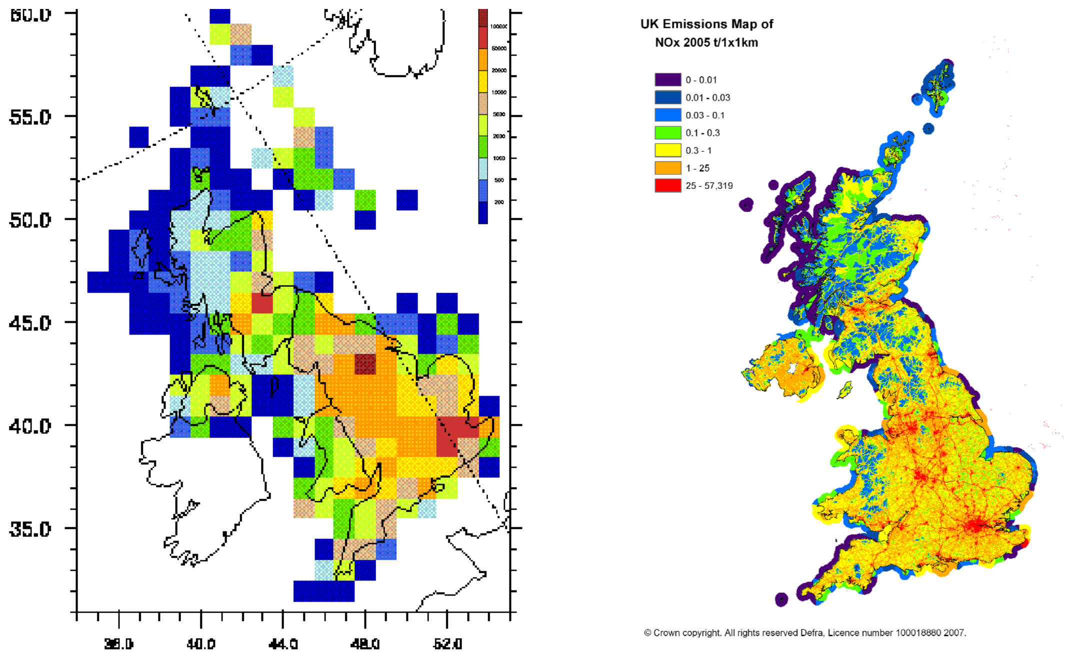

Fig. 1. Comparison of 50×50 km (left) vs. 1×1 km (right) resolution emission inventory of nitrogen oxides for the UK.

Source: EMEP Centre on Emission Inventories and Projections (http://www.ceip.at/) and UK National Atmospheric Emission Inventory (http://naei.defra.gov.uk/)

2. METHODS

2.1. Main drivers of spatio-temporal variations of input data

The majority of air pollutant emissions are directly driven by human activities, for instance the release of carbon dioxide, sulphur dioxide and nitrogen oxides due to the combustion of fossil fuels, or the emission of volatile organic compounds from paint and adhesive application. On the other hand, natural and biogenic processes contribute emissions to air predominantly driven by meteorological parameters such as temperature or precipitation. In addition to these more clear-cut cases, some human activities are closely linked to meteorology and climate, for instance in agriculture, leading to temporal emission patterns that are influenced by a mix of drivers.

From a sectoral perspective, the following classification can be derived:

- *Mainly driven by anthropogenic activities:* power generation, industrial processes, solvent use (both industrial and household application of paints, glues etc.), road transport, waste management & disposal
- *Mainly driven by meteorology:* natural and biogenic emissions
- *Mixed cases:* agriculture, household combustion

For the first category, statistical information of fuel consumption or activity patterns (e.g. on traffic levels, working hours, product sales) can be used to derive reliable temporal emission profiles. In most cases, this information is publicly available, albeit typically with a time-lag, so it is suitable for ex-post calculations, but information for future scenarios is often not readily available.

Fig. 2 shows exemplary variations in activity rates for road transport based on UK data.

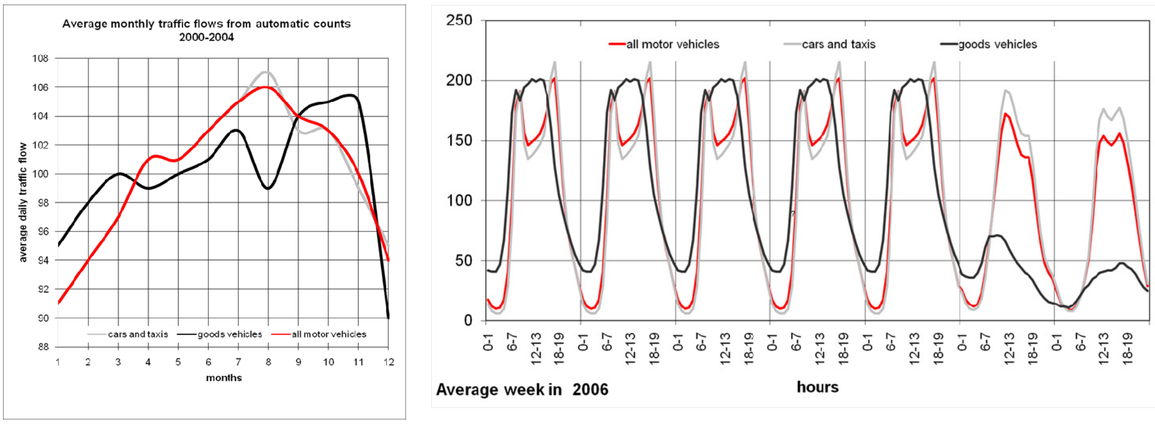

Fig. 2. Exemplary temporal profiles for road transport activities in the UK based on official statistics. On the left, the variation of passenger vs. freight transport is shown for an average year, on the right, a weekly profile is displayed, showing the clear differences between weekdays and weekends and the daily morning and afternoon peak due to commuting.

Source: UK Department of Transport Statistics (http://www.dft.gov.uk/statistics)

2.2. Requirements for spatially and temporally explicit model results

From a scientific point of view, improving input data for modeling has obvious merits, but there are other aspects that determine a strong need for a better representation of in particular temporal profiles of emission data. The results of atmospheric dispersion models are increasingly used to design and assess the impact of air pollution control policies. In most cases, exceedances of limit values are strongly episode driven, for instance when exceedances of hourly average concentrations of particulate matter are concerned (X days above a certain value) or the exposure of crops and ecosystems to high ambient concentrations of ground level ozone (accumulated exceedance of X ppb in ppb.days). These indicators are sensitive to model input data having an accurate hourly, daily or seasonal profile, to ensure that emissions are introduced into the model not only at the right location, but also at the right time.

In a similar way, the validation of modeling atmospheric concentrations of pollutants, or their deposition, by comparing model results with ground observations or remote sensing can be seriously affected if emission data are provided with inaccurate temporal profiles. Concentration peaks at the wrong time are penalizing model performance vs. observations as the typical comparison of bias or correlation will show model peaks not coinciding with observed peaks.

3. DISCUSSION

3.1. High resolution equals better models?

There is a general misconception that increasing the resolution, temporally and spatially, automatically leads to better – i.e. more accurate - model results. While this may be intuitive, it heavily depends on the availability of and accessibility to detailed input datasets. In most cases, the statistical and other information required to achieve the higher resolution is subject to assumptions and generalizations that need to be factored in when for instance uncertainty quantification of model results is conducted.

In many cases, bottom-up calculations are used to create emission inventories, with detailed information for instance on the vehicle stock, technologies and activity patterns (annual mileage, speed distributions etc.) being used in the calculation of emissions and further aggregation to sectoral annual emissions. However, these bottom-up figures, while being very detailed and disaggregated, are not “real” emissions, they are themselves model results where the vehicle fleet and its technological composition and its activities are used to derive a representation of an emission topography for a specific time frame. In contrast, the “real” emissions could only be determined by on-board online monitoring of each individual vehicle at all times in all conditions, which is obviously hard to achieve, both technically and logistically, and equally economically infeasible.

In addition to the generation of input data, the validation vs. real-world observations is a challenge, as the availability of observations in space and time is often sparse and in itself faces a lot of restrictions as to the representativeness for a given time or spatial scale.

Similar arguments are valid for other input data as well, for instance meteorology and the atmospheric processes (physical transport and chemical transformation).

The often posed question about what resolution could be ultimately achieved may thus be misleading and the more relevant question would be that of what is the most appropriate resolution for a specific scale (see section 4.1).

3.2. What do we gain?

In the view of the challenges in quantifying "improvement" the valid question is if (and what) we gain by the additional effort in creating more temporally and spatially resolved input datasets. Apart from the obvious drivers to represent the real situation in our models as best as we (economically) can, eliminating sources of uncertainties as such is a strong motivation. At this stage, it is often difficult to determine, due to which components a mismatch between observations and model results may occur. As a result, models are at times "tuned" to better match observations on the basis of the assumption, that processes are over- or underestimated within the model formulations. Even assuming perfect observations, the potential role of input data in driving model performance vs. process understanding being the cause for agreement or disagreement between modeled and observed values is obvious.

In this context, we can determine the main drivers for specifically addressing emission input data as follows:

- Emissions, their location, their amount and the temporal pattern of their release into the atmosphere are one of the main components of atmospheric modeling and the potential impact on model results is substantial.
- In parallel to further improving the process understanding and other aspects, such as meteorological drivers and global climate change, improving the representation of emissions in models in all dimensions is key to determine the causes of divergences between model results and observations.
- Having a better understanding of the temporal and spatial patterns of emissions can aid the design of monitoring strategies and validation experiments.

4. CONCLUSIONS AND OUTLOOK

4.1. Finding the appropriate degree of resolution

As briefly discussed in 3.1, the debate on what is technically or economically feasible is often clouding the fact that the capability of a model to predict or represent real world processes is often determined by the availability of data first and foremost. By creating more detailed and spatio-temporally explicit datasets, which rely on a wide range of underlying assumptions, model results do not improve per se and further uncertainties may be introduced in the process of creating the highly resolved datasets, which are not easy to quantify (see as well Oxley *et al.*, 2011a, b and Oxley and ApSimon, 2011).

Issues of scale apply as much to the modeling itself, as to the input data required and for lack of a better word, the appropriate scale and model for a specific science or policy question should determine the degree of spatial and temporal resolution. This means, that for a model looking to represent a European or hemispheric scale, at resolutions of 50 × 50 km or 100 × 100 km, the need for emission data in a high resolution of 1 × 1 km and hourly time steps is likely not required. At the same time, any expectations that such a model would accurately predict concentrations at the fine (urban or landscape, for instance) scale have to be rejected. On the other hand, local or urban scale models aiming to reproduce the specific concentrations at curbside or at local hotspots, both with regard to the exact timing and location of their occurrence, will require emission data with high spatio-temporal resolution (see for instance the results of a model intercomparison conducted by the UK Department of the Environment, Food and Rural Affairs http://uk-air.defra.gov.uk/research/air-quality-modelling?view=intercomparison).

However, while models are regularly applying nesting techniques to link between scales, the generation of emission datasets is typically less flexible and advanced. This is not surprising, as most emission datasets are not generated primarily with their use for modeling in mind, but rather as a means for reporting and compliance monitoring in legal/political frameworks (e.g. national emission reporting obligations for the EC National Emission Ceilings Directive or the UNECE Convention on Long-Range Transboundary Air

Pollution). In this context, emissions by administrative or national boundaries are of most interest and the time scale is most often annual. Spatial and temporal distribution of emissions thus generated is often applied at a later stage, not always having the full knowledge of what data have been used to create the emission dataset in the first place. A selected few datasets exist, which are generated from bottom up with the primary objective to serve as input to atmospheric modeling. These purpose-built inventory datasets typically come with a specific scale – determined by the modeling activities for which they were created.

From the view of generating model input data, there would be merit in considering a paradigm change towards storing primary data from which emissions can be generated in different temporal or spatial scales, rather than in the current inventory formats with fixed spatio-temporal domains. For those tasked with generating the inventory datasets, this would not even require additional efforts, as in most cases current inventory generation is based on the same data in delivering bottom-up emission estimates. Having access to this level of information, atmospheric models or emission-preprocessors could generate emission input data at the scale required for a specific modeling activity on the fly. Different aggregation levels could be achieved in the same way.

The above applies first and foremost to anthropogenic emissions that are mainly activity driven. For fully or partly meteorology driven emissions, online-generation within atmospheric models, using the same meteorological input data that drive the dispersion and transformation, is the most appropriate way in generating emissions. As this is directly built into the atmospheric models, spatial scale and time steps are in most cases already at the same level as the models.

4.2. Next steps

Data availability is one of the key limiting factors for deriving detailed emission inventories. For the spatial distribution, proxy variables such as population density or explicit geographical information on road networks or the location of large point sources can provide a sufficiently detailed dataset to create maps. For temporal profiles, statistical information on fuel and energy use, working patterns and other activity data can be used to derive sufficiently detailed patterns for key emission source sectors. Yet, this kind of information is time consuming to collect and not always freely accessible. Even if it is, statistical data in most cases is gathered and made available with a time lag of a few years, which impedes modeling of current or recent years and adds a degree of additional uncertainty to modeling scenarios for the future. The latter is difficult to overcome, as creating robust scenarios of future activities e.g. on an annual level is already challenging, anticipating temporal patterns will be even more difficult when drivers such as global climate change may introduce changes in behavioral patterns.

To overcome the issue of a time lag in gathering information for current periods, the increasing availability and quality of earth observation (EO) products may provide opportunities to apply model-data-fusion, including EO and ground based measurements with atmospheric models. This combination of different datasets and models could bridge the gap between the few monitoring sites providing highly temporally resolved measurements, the larger number of stations providing monthly or annual measurements and the need of atmospheric models for hourly or at least diurnal variations.

In a similar way, the increasing availability and economical feasibility of deploying larger numbers of sensors and collecting their data (near) real time can help to for instance model atmospheric concentrations for field campaigns in parallel to the measurements, with more accurate input data on the temporal patterns of emissions and/or activities to ensure that the model does indeed “see” the same environmental conditions as picked up by observations.

Last, but not least, while the above applies to all sectors where human activities are predominantly driving emission patterns, the need for more sophisticated approaches to derive such patterns for sources such as agriculture, including the influence of meteorological factors, is vital. There is a potential conflict between the need to provide emission inventories for compliance monitoring purposes, based on – often rigid – rules that are necessary to make emissions comparable over time and measure progress against a set of targets, and the need to provide input to models that represents a realistic pattern of emissions. Introducing for instance functions modifying the release of ammonia or nitrous oxides from agricultural soils due to temperature may lead to annual emissions that are above (or below) the statically calculated official inventory figures. There are ways to avoid this conflict by setting targets based on a specific year or range of years to account for the meteorological influence in harmonizing emission inventories. While this is technically feasible, it adds a level of complexity to the political negotiations of emission targets, which - at this time - may be difficult to justify.

It is thus important to provide first and foremost a robust message to policy decision makers on the sensitivity of the model results towards variations in both temporal and spatial profiles of emission data. Secondly, developing and testing robust methods to generate appropriate degrees of resolution for the scales models are applied on and quantifying the – change in – uncertainties involved in this part of atmospheric dispersion modeling will deliver evidence to inform the policy process.

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