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The innovative concept of three-dimensional hybrid receptor modeling

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HIGHLIGHTS

- Three-dimensional PSCF and CWT for identification of source altitude distribution.
- New hybrid receptor model for pollutant altitude distribution along transport pathway.
- Refined approach for more realistic representation of source distribution.
- Potential $PM_{2.5}$ source regions were registered in Romania, Bulgaria and Bosnia.
- Pollutant time series preprocessing to make models applicable for urban sites.

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ABSTRACT

The aim of this study was to improve the current understanding of air pollution transport processes at regional and long-range scale. For this purpose, three-dimensional (3D) potential source contribution function and concentration weighted trajectory models, as well as new hybrid receptor model, concentration weighted boundary layer (CWBL), which uses a two-dimensional grid and a planetary boundary layer height as a frame of reference, are presented. The refined approach to hybrid receptor modeling has two advantages. At first, it considers whether each trajectory endpoint meets the inclusion criteria based on planetary boundary layer height, which is expected to provide a more realistic representation of the spatial distribution of emission sources and pollutant transport pathways. Secondly, it includes pollutant time series preprocessing to make hybrid receptor models more applicable for suburban and urban locations. The 3D hybrid receptor models presented herein are designed to identify altitude distribution of potential sources, whereas CWBL can be used for analyzing the vertical distribution of pollutant concentrations along the transport pathway.

1. Introduction

Air mass trajectory analysis has been widely used to study dynamical processes and pollutant circulation patterns in the atmosphere. Over the last few decades, a variety of statistical tools have been developed and applied for analyzing a large set of trajectories, including general hybrid receptor models that are focused on the behavior of ambient pollutant at the point of impact (Hopke, 2003). The receptor-oriented models based on conditional probability and residence time analysis, such as potential source contribution function (PSCF) and concentration weighted trajectory (CWT), have been used in numerous air pollution studies to investigate the spatial distribution of potential emission sources and assess their impact on single receptor location without using emission inventories (Brereton and Johnson, 2012; Byčenkienė et al., 2014; Sen et al., 2016; Li et al., 2017). PSCF relates residence time of trajectory segment endpoints in a potential source area with the above-threshold pollutant concentrations at the receptor site (Ashbaugh et al., 1985). However, because PSCF has difficulties distinguishing strong sources from moderate sources, it was modified into the CWT (Hsu et al., 2003) which has the additional ability to determine the relative significance of potential sources by calculating concentration gradients.

The conventional approach to hybrid receptor modeling has several drawbacks. To our knowledge, the concept of hybrid receptor modeling estimates the relative importance of transport

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processes without respecting the differences between background and urban receptor locations. Therefore, we propose time series preprocessing to make hybrid receptor models more applicable for suburban and urban sites, where the pollutant concentrations are dominated by local emissions. Another disadvantage of the conventional approach is that computing the trajectories for predefined arbitrary chosen heights at the receptor site does not necessary yield a realistic representation of pollutant transport pathways because it overlooks the fact that the redistribution of emitted pollutant species occurs dominantly at the lowest 100 to 3000 m of the atmosphere, a part known as planetary boundary layer (PBL). According to Stull (1988), pollutant ambient concentrations exhibit a significant decrease with height because the species emitted or generated near ground are mostly trapped and concentrated within the PBL, whereas free atmosphere concentrations remain low. Therefore, in this study we considered the PBL height fluctuations for more realistic evaluation of source-receptor relationships in air pollution analysis, not only at the receptor site, but also at each segment along the transport pathway. Given that non-PBL transport of pollutants is relatively rare (Langford et al., 2015), but observed for certain cases, such as intercontinental transport and Arctic Haze, the current approach of computing the trajectories for predefined heights, as described in the work of Cheng et al. (1993), is more appropriate for these occasions.

In order to obtain a more realistic description of transport processes, we introduce the innovative approach to air pollution transport analysis based on backward trajectories, which accounts for meteorological factors that govern the vertical distribution of pollutant concentrations and appreciates the differences between background and urban locations. To that end, a three-dimensional (3D) improvement of the conventional PSCF and CWT models, as well as new hybrid receptor model that uses a 2D grid and a PBL height as a frame of reference are presented.

2. Air pollutant transport phenomena

Discriminating the relative importance of background, local sources and transport processes for pollutant concentrations at the sampling site is one of the key issues in air pollution analysis. The conventional concept of hybrid receptor modeling takes into account the concentrations greater than the arbitrary chosen criterion value (*e.g.* mean or median concentrations), thereby assuming that individual peaks in the pollutant time series are mainly observed as a result of regional or long-range pollutant transport (Kassomenos et al., 2006; Grivas et al., 2008). While this approach may be considered appropriate for background sites where sudden rise in concentrations can be almost exclusively observed as a result of transport, it may fail for suburban and urban locations. Conversely, we assume that in suburban and urban areas, dominated by a number of local emission sources, transport and background jointly contribute to gradual variations of a concentration base level, whereas the superimposed pronounced peaks in pollutant time series are registered as a result of local emissions (Fig. 1a). Following this logic, differentiation between the contributions of local and remote emission sources was obtained by a two-step procedure that was described in our previous studies (Stojić et al., 2015a, 2016).

In brief, for excluding the contribution of local sources from the time series, baseline. rollingBall from the "baseline" package (Kneen and Annegarn, 1996) in statistical software R (Team R.C., 2013) was chosen out of a number of functions available for baseline extraction. Subsequently, Trajectory Sector Analysis (TSA) was applied to the derived baseline to distinguish between the contribution of background and transport, and the obtained transport time series were further used as input data for hybrid receptor models.

The potential concept of 3D PSCF analysis has been recently proposed by Kim et al. (2016). As defined in this study, an air parcel passing through a cell with an emission source was considered to be unaffected by pollution if it passes at an altitude higher than the arbitrary threshold of up to 3000 m. Therefore, the authors calculated the PSCF by simply ignoring the segment endpoints above the chosen threshold value. However, as previously mentioned, the troposphere extends from the ground up to 11 km, but only the lowest part or the PBL is directly influenced by the underlying surface and responds to surface forcing (Stull, 1988). As the pollutants emitted from the ground are dominantly trapped and dispersed within the PBL by turbulent mixing under favorable meteorological conditions, the near-surface pollutant concentrations registered at the receptor site could correspond to atmospheric concentrations only within the PBL height. In compliance with this, the previous studies (Gan et al., 2011) that used the community multiscale air quality (CMAQ) modeling system to simulate the emission, transport, transformation and deposition of atmospheric pollutants have shown that pollutant concentrations rapidly decrease in the vicinity of the PBL (Fig. 1b). The PBL height exhibits diurnal variations in a broad range from several tens to several thousands of meters, and therefore, the 3D analysis that relies on a set of trajectories obtained for a single predefined height does not adequately address the issue of pollutant transport. Unlike the study of Kim et al. (2016), as well as other studies that use the conventional hybrid receptor models, the transport analysis presented herein accounts for hourly PBL height fluctuations by including the trajectories based on their representativeness. Namely, the dynamic calculation of trajectories was performed within the PBL at the receptor site. The trajectories with endpoints exceeding PBL height for 20–50% depending on height (due to uncertainty in the PBL height determination, according to Seidel et al., 2012) were excluded from the analysis. Additionally, due to the emergence of significant turbulences within the PBL, trajectories can be quite curved, and disruption can occur at the bottom level, which is often the case for small height-trajectories above the receptor site. Such trajectories were excluded from the analysis as they do not properly represent transport.

2.1. 3D PSCF

The contribution of a specific source to pollutant concentrations at the receptor site is considered to directly correspond to air mass residence time over the region where the source is located (Dimitriou and Kassomenos, 2014). The endpoints along the trajectory separated by a specific time period are used to calculate air mass residence time for each grid cell. As described by Hopke et al. (1993), if N is the total number of trajectory endpoints, the probability that n trajectory endpoints fall into the ijth cell (n_{ij}) is given as:

$$P\left[A_{ij}\right] = \frac{n_{ij}}{N} \tag{1}$$

If we assume that the same ijth cell contains a subset of m_{ij} endpoints for which the corresponding trajectories arrive at the receptor site when the transported concentrations are higher than the predefined criterion value (*e.g.* mean value), the probability of high concentration event B_{ij} is given by: