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Effects of downscaled high-resolution meteorological data on the PSCF identification of emission sources☆

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HIGHLIGHTS

- Impacts of PBL parameterization and grid resolution on PSCF modeling were studied.
- Dynamically downscaled WRF data used as input to HYSPLIT and PSCF modeling.
- Use high-resolution meteorological data recovered missing sources of black carbon.
- The MYJ PBL parameterization performed consistently in multiple grid resolutions.

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ABSTRACT

The Potential Source Contribution Function (PSCF) model has been successfully used for identifying regions of emission source at a long distance in this study, the PSCF model relies on backward trajectories calculated by the Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model. In this study, we investigated the impacts of grid resolution and Planetary Boundary Layer (PBL) parameterization (e.g., turbulent transport of pollutants) on the PSCF analysis. The Mellor-Yamada-Janjic (MYJ) and Yonsei University (YUS) parameterization schemes were selected to model the turbulent transport in the PBL within the Weather Research and Forecasting (WRF version 3.6) model. Two separate domain grid sizes (83 and 27 km) were chosen in the WRF downscaling in generating the wind data for driving the HYSPLIT calculation. The effects of grid size and PBL parameterization are important in incorporating the influence of regional and local meteorological processes such as jet streaks, blocking patterns, Rossby waves, and terrain-induced convection on the transport of pollutants by a wind trajectory. We found high resolution PSCF did discover and locate source areas more precisely than that with lower resolution meteorological inputs. The lack of anticipated improvement could also be because a PBL scheme chosen to produce the WRF data was only a local parameterization and unable to faithfully duplicate the real atmosphere on a global scale. The MYJ scheme was able to replicate PSCF source identification by those using the Reanalysis and discover additional source areas that was not identified by the Reanalysis data. A potential benefit for using high-resolution wind data in the PSCF modeling is that it could discover new source location in addition to those identified by using the Reanalysis data input.

1. Introduction

Identifying emission sources is of great interest to international treaty for mitigation of climate change in the Arctic. There are instances where an emission source inventory does not exist and the source location is impractical to know *a priori*. Inversion technique is therefore undertaken for emission source identification and apportionment. The complexity of solving the inverse problem of source identification and attribution has been well-known to the field of environmental chemistry and air quality management

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(Cheng and Hopke, 1986a; 1986b; Hopke, 1985, 1991; Fleming et al., 2012) and nuclear forensics (Anderson-Cook et al., 2015), for example. In general, there is no single solution to the inversed problem.

To estimate source emission factors by an inversion technique, a large solution uncertainty could exist due to the condition imposed on the solution. For example, the number of sources (the unknowns) may be more than the number of measurement data (the knowns) that results in multiple possible solutions and large uncertainty about each solution. There may be cases where the number of sources is more than the number of available material signatures leading to an under-determined system of equations. In other words, there are more than one solution that can meet the needs of the equation system.

Alternatively, for identifying the geographic location of a source or sources (of material signatures) using an inverse atmospheric modeling approach, one may use backward wind trajectory. Among which the Potential Source Contribution Function (PSCF) model (Cheng, 2014; Cheng and Lin, 2001; Lin et al., 2001) is one such approach, and the PSCF has been successfully used over the past two decades for air quality resources management at spatial scales ranging from the metropolitan scale (Gao et al., 1994; Cheng et al., 1993a) to continental (Cheng and Lin, 2001) and hemispherical (Cheng et al., 1993b; Cheng, 2014). The PSCF model derives a geographical map showing the probability of grid cells of known latitude and longitude coordinates. A grid cell of high PSCF value (>0.8 for example) indicates the cell or area is very likely to be the source of the emitted material. At its present formulation, PSCF does not provide a quantitative measure of the emission factor of that identified grid cell.

It has been reported that the accuracy of a backward wind trajectory is dependent on the accuracy of available meteorological data (e.g., wind direction, wind speed, humidity, etc.) (Kahl and Samson, 1986, 1988). The mechanics of computing the backward trajectory is straightforward, but the uncertainty at each endpoint can accumulate through each time step backward in time into an error so large that it becomes unrealistic at the end of a long (e.g., 10-day) backward trajectory. The accumulation of numerical errors in the model enumeration could be from factors such as input data errors due to instrument malfunction or out of calibration, lack of key meteorological data over a large area such as the Arctic or over the Atlantic and Pacific Ocean, representativeness of the model process parameterization and model grid resolution. Since a backward trajectory has to travel a large distance in a hemispheric PSCF analysis, investigation on the effects of the trajectory caused by uncertainty in the wind data, which is coupled to Planetary Boundary Layer (PBL) processes as well as the representation of them over a long distance (several thousand kilometers), is required.

For example, topography, type of surface elements (water body, vegetation, sand, ice, etc.), and man-made structures can all affect the three-dimensional movement of a trajectory backward in time in the atmosphere. These land attributes affect surface-atmosphere exchange of heat (sensible and latent) and momentum (mass like CO_2, water vapor, particulate matter and trace gases), which play an important role in the genesis and life cycle of boundary-layer turbulence controlling the vertical transport and mixing of pollutants. All these boundary layer processes are typically parameterized in so-called PBL schemes for a modern weather model. There are more than a dozen PBL schemes available in the Weather Research and Forecasting (WRF) model (Skamarock et al., 2008) ARW core.

Trajectory calculations using meteorological data are constrained by spatial and temporal resolution. Kahl and Samson (1986, 1988) have investigated the impacts on the trajectory of the uncertainty of meteorological data used. They suggested accuracy of the trajectory operating at a mesoscale can be improved by an increased spatial resolution. Regularization of the meteorological data is typically done through a process called Reanalysis such that meteorological data are in uniform format and quality controlled for further use. The Reanalysis data were provided in a spatial resolution on a model domain grid size of 250 km by 250 km. Many micro- and meso-scale atmospheric processes; e.g., hurricane and vertical up-draft, that can significantly affect the trajectory movement but cannot be adequately simulated when a domain grid size is coarse. Thus, it is also likely that the trajectory endpoint can be effected by the domain grid size.

Since WRF-ARW was used to derive high-resolution wind data for driving the Hybrid Single-Particle Lagrangian Integrated Trajectory model (HYSPLIT; Draxler, 1999) backward trajectory calculation, we investigated the effects of model domain grid size and choice of PBL scheme on the accuracy of the computed backward trajectory. We compared the PSCF results that were based on the trajectories calculated from the WRF meteorological data, against the one performed by NCEP/NCAR Reanalysis used earlier in Cheng (2014) and showed how the effects eventually propagated and impacted the PSCF outcome and, therefore, the end results of source identification.

2. Description of ambient sampling sites and ambient data

Black carbon (BC) data, obtained through the Canadian NAtChem portal and used in the PSCF analysis, were from ambient air filter samples collected at Alert, Nunavut, Canada ([82.5°N, 62.3°W] at a height about 200 m above mean sea level) and analyzed by Environment Canada. Hirdman et al. (2010) described extensively the long-term trends of black carbon in the Arctic, and change in the atmospheric transport. Fig. 1 shows the location of the Alert sampling site in the Arctic Circle. The Alert station has a long, remarkable history contributing to the understanding of Arctic haze and of air chemistry in cold climates since the 60s (Barrie et al., 1985; Sharma et al., 2004). The details of sample collection, analysis, and quality control of the NAtChem data can be found in Sharma et al. (2004) and will not be repeated here.

BC concentration from the year 2000 was measured by an aethalometer (McGee model AE31) on an hourly interval for this analysis. The BC data are displayed in a box-whisker plot for each month in 2000 in Fig. 2. The 75th percentile lines with the top of the box, the middle line is the 50th percentile (or median), and the bottom of the box is the 25th percentile of the hourly BC data. Data larger than the 95th percentile values are displayed as points outside the whisker. The seasonality of the BC data is clearly shown in Fig. 2; winter or dark season has higher BC concentration, while summer or light season has lower BC concentration. This seasonal pattern is consistent with those for other Arctic Haze species reported in the past (e.g., Shaw, 1995; Barrie, 1985; Cheng et al., 1993b).

3. Description of selected PBL schemes

Turbulent mixing within the lower troposphere is needed to transport pollutants from emission sources to a distance far away. Turbulence is mostly a subgrid-scale process, but its presence in the PBL directly modulates a simulation's depiction of mass fields relevant for transport problems. Each scheme represents mixing on a local and/or nonlocal basis (Hines and Bromwich, 2008). Local schemes only consider immediately adjacent vertical levels in the model, whereas nonlocal schemes can consider a deeper layer covering multiple levels in representing the effects of vertical mixing through the PBL. To investigate the effect of grid size and PBL on the computed trajectories, we chose two schemes: the MYJ