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Hybrid modelling approach for effective simulation of reactive pollutants like Ozone

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HIGHLIGHTS

- Paper shows limitations of deterministic models to predict extreme concentrations.
- Hybrid modelling technique is used to predict entire range with improved accuracy.
- Hybrid model is demonstrated to predict concentrations of reactive species (Ozone).
- Paper shows improvement in results using hybrid model over deterministic models.

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ABSTRACT

Prediction of air quality is an important component of any air quality management programme. Broadly, two approaches are used to predict the ambient air quality – the deterministic and the statistical approach, with each approach having its own merits and demerits. While the models based on the deterministic approach accurately predict the concentrations of air pollutants in the middle percentile range, the statistical models provide a better estimate of concentrations in the extreme percentile ranges. However, the statistical models are site specific and are not able generate 'what-if' scenarios; the deterministic models on the other hand are general in character and useful in creating alternative scenarios. An alternative approach – hybrid modelling is a technique which aggregates the benefits of the two techniques and predicts the 'entire range' of the distribution. While in the past there were attempts to predict the concentrations of inert pollutants using hybrid modelling approach, this paper shows the hybrid model applications for reactive secondary pollutants like ground level Ozone (GLO). This study presents the development of a hybrid model that concatenates the results of CMAQ (community multi-scale air quality model) as its deterministic component with statistical distribution model (based on the specific area category and timeframe) to predict the entire range of GLO concentrations. Predictions have been made using both purely deterministic and hybrid approaches at a receptor location near a major traffic intersection. The performance of the model has been found to improve from an index of agreement from 0.77 (deterministic model) to 0.91 (hybrid model). In order to assess the predictive capability of the hybrid approach, the model has been tested at an entirely different location for different set of temporal data. The results show an improvement in the predictions using the hybrid model over the deterministic model.

1. Introduction

Air pollution has been an important problem since developmental activities grew at a rapid pace. While average concentrations may have long term chronic health effects, extremely high concentrations even for small duration can have serious health implications. Hence, air quality management plan needs to be developed which takes into account not only the middle ranges of pollution levels but also the extreme values. Prediction of air quality using models is therefore an important component of any air quality management plan. The air quality 'predictor' for pollutants can be developed either deterministically or statistically. The traditional deterministic models are causal in

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nature and simulate the major atmospheric processes that affect the air pollutants. Though computationally more expensive, these models provide direct linkages between source emission and resultant ambient air pollution along with interrelationships among multiple pollutants (Cai et al., 2008; Mathur et al., 2008; Yu et al., 2003, 2004, 2008; Chuang et al., 2011). These models require detailed source emission inventory and meteorological data. While the process-physics based deterministic air quality models prove good to predict concentrations in the middle ranges, they fail to predict extreme values effectively (Sharma et al., 2012; Khare and Sharma, 2002; Jakeman et al., 1988). The alternative statistical models on the other hand are not based on causal factors but are empirical in character and are based on the historical data. These are better suited to capture the past trends of the pollutants and back cast the pollutant concentration and predict extreme concentrations with more accuracy. The statistical distributional form, fitting to the concentrations data, is based upon several factors, i.e. source types, pollutant types, emission patterns, meteorological conditions, and averaging times (Taylor et al., 1986). However, the processes in the atmosphere may differ depending upon the area category of the study domain (residential, kerbside, industrial, background/urban/rural). As the preparation of an air quality management plan requires knowledge of both middle and extreme ranges of pollutants (Gokhale and Khare, 2005), hybrid modelling could be one of the solutions to this problem which can predict the entire range based on both deterministic and statistical modelling approaches. Hybrid modelling is a technique which aggregates the benefits of the two techniques and predicts the 'entire range' of the distribution. Although, some work has been done in the past for predicting pollutants which are inert in nature like carbon monoxide (CO), there is tremendous scope of research in developing and applying models based on the hybrid approach for prediction of reactive species like oxides of nitrogen and GLO. The present study aims to develop a predictive air quality model for the entire range of GLO concentrations based on the hybrid approach.

2. Materials and methods

2.1. Site description

Delhi was selected as the study domain for the current work. Continuous air quality monitoring of GLO is carried out at three monitoring stations in Delhi. ITO (Income tax office) and DCE (Delhi College of Engineering) monitoring station were selected for the testing and verification of the hybrid model approach (Fig. 1).

The choice of the two stations was based on the differences in their emission profiles. ITO monitoring site is a traffic intersection having very high vehicular density, while DCE is a location in the outskirts of the city, having significantly lesser vehicular activity. The surrounding landuse around the ITO monitoring station is predominantly institutional which attracts large volume of traffic. Moreover, the traffic intersection links the four important roads of the city and caters to heavy traffic loads. Around 0.15 million vehicles pass through the intersection daily and contribute to the deterioration of air quality. The site continuously shows violation of ambient air quality standards during a year. On the other hand, DCE monitoring station lies towards the north end of the city. The station lies in an institution surrounded by residential areas. Vehicular activity is comparatively less and hence lesser ambient concentrations of the primary pollutants like particulate matter (PM), oxides of nitrogen (NO_x) etc. are observed at the monitoring site. However, the ozone concentrations were found to be higher at DCE than ITO because enhanced destruction of ozone at ITO due to its reactivity with primary nitric oxide (NO) released from the vehicles. The striking differences in the landuse, source emission profiles and monitored ozone concentrations lead to the selection of the two sites for testing the hybrid modelling approach.

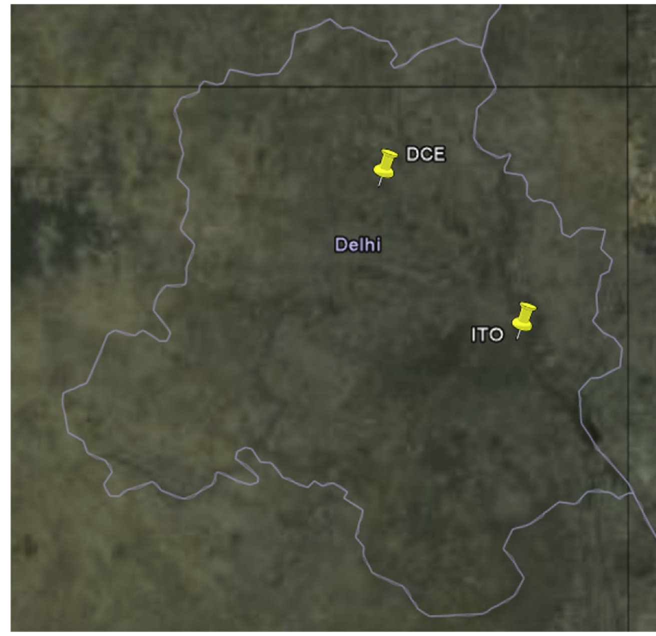

Fig. 1. Location of the two monitoring sites in Delhi (ITO and DCE). Source: Google Earth, 2013

2.2. Data description

Emission inventory for Delhi is prepared based on the GAINS Asia framework (URL: http://gains.iiasa.ac.at/index.php/gains-asia). Information about the number of vehicles, power plants, domestic fuel usage, industries etc. was collected and relevant emission factors were used to estimate the emissions for the year 2010. The emissions are spatially distributed based on grid-wise distribution of emissions in CPCB, 2011. NCEP data (www.ncep.noaa.gov/) has been downloaded for the year 2010 for the study domain which served as an input to the WRF (www.wrf-model.org/) model to generate meteorological fields. Other than this hourly Ozone data has been collected from CPCB (www.databank-cpcb.nic.in/) for two monitoring stations (ITO, and DCE), which was later used to develop the statistical model for extreme values prediction.

3. Methodology

The development of hybrid model involves four steps (Jakeman et al., 1988) – construction of deterministic model; identification of best-fit statistical distribution model (SDM) for the observed air quality data; estimation of parameters of the identified SDM using the censored data generated by the dispersion model in the middle percentile range; and prediction of pollutant concentration in the entire range of the distribution. The step wise methodology is explained below.

The deterministic models generally are able to accurately predict the concentration in the middle percentile ranges, often referred as the reliable range. Therefore, the first step involves application of an appropriate causal deterministic model that uses source emission and meteorological data for generating the pollutant concentrations. The output of the deterministic model is censored for picking up the data in the reliable range. For the present study, the Community Multi-scale Air Quality (CMAQ), which is a three-dimensional chemical transport model, has been