The modelling framework for this study consists of a meteorological model, an air quality model and an emission inventory database which were integrated to simulate the local and regional atmospheric circulation and predict the pollutant concentrations on national level. Ambient PM$_{2.5}$ concentrations were simulated in this study using the WRF-CMAQ modelling combination. Models-3/CMAQ modelling system has been used in the study to assess chemical transport of different pollutant species under prevailing meteorological conditions (Byun and Ching, 1999). The CMAQ system is based on multi-pollutant and one atmosphere approach and is a leading air quality model used for assessment of ozone (O$_3$) and aerosols (Byun and Schere, 2006). CMAQ is known to have certain advantages over the traditional Gaussian-based models (ISCST3, AERMOD), which have been generally used in India in source apportionment studies. CMAQ is Eulerian model as compared to Gaussian approach followed in AERMOD/ISCST3 and includes many more atmospheric processes than traditional models. CMAQ deals with chemical reactive species such as ozone, NO$_x$, hydrocarbons, and secondary particulates (sulphates, nitrates) and can be used on a range of spatial scales—continental to local, and accounts for long- and medium-range transport of pollutants. The model can deal with multiple pollutants together rather than individually and also takes into account the photochemistry which is not accounted for in traditional models.

A number of studies have shown satisfactory performance of the Community Multi scale Air Quality Modelling System (CMAQ) to predict urban- and regional-scale concentrations of a variety of pollutants (Marmur et al., 2009; Jose et al., 2013; Liu, 2013). The model has been extensively used for policy and research evaluations across the world (Paza et al., 2013 (Mediterranean Basin); Sokhi et al., 2006 (London); Chen et al., 2007 (Beijing); Khiem et al., 2010 (Japan); Simon et al., 2012 (USA). Sharma et al. (2014) have applied the CMAQ model to predict NO$_x$ concentrations for Bangalore city and ozone concentrations in India (Sharma et al., 2016). Based on the widespread applicability and requirements of multi-pollutant prediction, WRF (ver 3.1.1)-CMAQ (ver 5.0.2) combination have been chosen for carrying out the assessment in the present study (Figure 17).

WRF model runs have been carried out to generate three-dimensional meteorological fields over the study domain which acts as an input to the CMAQ model along with emissions inventory. ECMWF and USGS datasets have been used for running the WRF model, the output of which are the three-dimensional meteorological inputs that are fed to the CMAQ model.

India-scale emission inventory data at a resolution of 36 km x 36 km has been prepared in this study and has been provided as input to CMAQ model. To account for transport of pollutants from outside India, international boundary conditions have been adopted from global air quality products of NCAR (National Centre for Atmospheric Research, US). These global products are generated using the global chemical transport model MOZART. The emissions in neighbouring countries, such as Pakistan, Nepal,
Bangladesh, etc., which fall within the Indian study domain are taken from ECLIPSE database of IIASA (2014).

With these inputs, the model was run for the year 2016. The simulated ambient air concentration of PM$_{2.5}$ was validated with the selected annual automatic air quality monitoring stations data from the CPCB (www.app.cpcbccr.com). The validation of this model established that the model is able to reproduce physical and chemical processes which define pollutant concentrations, and it can be further utilized for running sensitivities of different sources.

The simulated results were validated against the observed measurements collected from the CPCB in the year 2016 with annual average concentration measured in major cities across India. The average ratio of simulated to observed values was found to be ~ 0.74 (Figure 18), which can be considered quite satisfactory. City wise variations in simulated and observed results attributed to, a) variations in landuse land cover pattern in different cities; b) the simulated value represents a single value over 36 km ×36 km area; whereas, observed values are generally the average of n numbers of monitoring locations in the specific city. These factors affects city wise variations in observed and simulated ambient PM$_{2.5}$ concentrations.

The spatial and temporal variation of simulated ambient PM$_{2.5}$ concentration over the Indian domain during 2016 (Figure 19) suggests dominance of internal sources during winter months which can be attributed to mainly two factors: i) agriculture residue burning, practised mainly by farmers of Punjab, Haryana and western Uttar Pradesh in the months of October and November. The ambient concentration of PM$_{2.5}$ over the region increased from the month of September to November and starts to dissipate in the month of December; ii) the meteorology, the wind conditions prevailing in winter are not conducive to dispersion due to slowdown in horizontal wind along with decrease in planetary boundary layer due to fall in ambient temperature (TERI, 2018). Further, burning of biomass is also prevalent for maintaining warmth in winter season both inside and outside of houses in the region, which also contribute significantly to ambient PM$_{2.5}$ concentration.
However, during the summer months the dominance of contribution from the western region outside the political boundary of India can be observed (Figure 19). This is attributed to the prevailing wind direction and higher wind speed compared to the winter months. Further, higher concentration of PM$_{2.5}$ is visible all over the year over the IGP region. This PM$_{2.5}$ concentration is washed down in the monsoon months, i.e., June and July.

The simulated monthly data also suggests that the PM$_{2.5}$ concentrations in most of the locations in India are above the annual average National Ambient Air Quality Standard of 40 µg/m$^3$ prescribed by CPCB (Figure 19). This is mainly high in the densely populated regions of India, such as Indo-Gangetic belt, Maharashtra-Gujarat region and parts of Orissa-Andhra Pradesh-Telangana-Karnataka-Tamil Nadu. This high concentration may be attributed to the sectors which are driven by the presence of people in any area, such as waste generation, crematoria, transport, residential, etc. While in scarcely populated regions, such as north east and Jammu and Kashmir, low level of PM$_{2.5}$ concentration is simulated round the year.

A few hotspots of ambient PM$_{2.5}$ concentrations (Figure 20) over Chhattisgarh and Odisha may be attributed to the presence of major thermal power plants and industries in this part of the country. The power and industry sectors remain in operation throughout the year, resulting in the release of high level of PM$_{2.5}$ levels in the region.

The regional variations in ambient PM$_{2.5}$ concentration during 2016, requires further study to know the seasonal variation of the sources in different regions to develop appropriate regional air quality management plan.

Figure 19 Spatiotemporal variations of simulated ambient PM$_{2.5}$ over the Indian subcontinent during 2016
Figure 20 Simulated annual average ambient $\text{PM}_{2.5}$ concentration ($\mu\text{g/m}^3$) in India during 2016