

Comparison of field monitored and prognostic model generated meteorological parameters for source dispersion modeling

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Abstract Comparisons were made between field monitored and prognostic model generated meteorological parameters for source dispersion modeling in Chandrapur, India. The first set of meteorological fields was generated using field monitored data based on measured parameters of SODAR and Mini-sonde. The second set of meteorological fields was generated using a prognostic model MM5 version 3.6.1. AERMET meteorological preprocessor was used to determine derived parameters from monitored and modeled parameters. Wind speed, wind direction, temperature, surface heat flux and mixing height were estimated separately for the two fields. Wind speed observed from SODAR was higher than the model predicted value. Temperature data from the Mini-sound was compared to MM5 modeled data and it was observed that MM5 under predicted temperature by 7 °C. Statistical measures indicated poor performance of the model. Results indicated that the use of prognostic models for predicting meteorology to study air quality in a region must be calibrated to local boundary conditions. There is a need to enhance data nudging and validation of prognostic models for different climatic conditions.

Keywords AERMET · Comparison · Meteorology · MM5 · Prognostic model · Sodar

Introduction

Source dispersion modeling is a widely used technique to predict the concentration of pollutants released from various sources like thermal power plants, automobiles and various other manufacturing units. Based on emissions inventories and meteorological parameters, a source dispersion model can be used to predict concentrations at selected downwind receptor locations. Meteorological parameters play a vital role in air quality dispersion models for accurate prediction of concentrations. The input meteorological parameters required for dispersion modeling are classified as surface and upper air parameters. These parameters are either monitored on the field or predicted by a prognostic model. Recent advances in numerical weather prediction models have enabled the use of the prognostic model viable for estimating meteorological parameters.

One of the main focuses on monitoring meteorological parameters is to represent the true atmospheric state of the site. Unfortunately, consistency in monitoring parameters requires advanced instruments and established practices. The upper air parameters are only monitored at some parts of a country and for remaining regions they are interpolated from data available at the nearest meteorological station. Even advanced instruments cannot measure the upper air data after certain altitude, thereby limiting their prospects. In such cases, a three dimensional prognostic model that solves the fundamental fluid dynamics and scalar transport equations can be used to predict meteorological parameters. Prognostic model eliminates the need to have site-specific meteorological observations to drive the air quality dispersion model.

Various studies have been carried out to assess the uncertainties in use of prognostic models for air quality assessments (Seaman 2000; Sistla et al. 1996, 2001; Pielke

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1998; Pielke and Uliasz 1998; Kumar and Russell 1996; Hogrefe et al. 2001). The topic of such meteorological model evaluation has been the focus of many air quality-related studies. Meteorological model evaluations center on how the model performs with regard to predicting surface-based measurements of temperature, wind speed, moisture, and precipitation (Gilliam et al. 2006). The point measurements of meteorological parameters are matched to the volume-averaged model results in space and time. Statistics such as mean bias, root-mean-squared error, mean absolute error, and index of agreement are then calculated and used as metrics to judge model performance (Gego et al. 2005; Vaughan et al. 2004; Mass et al. 2003; Tesche et al. 2002; Emery et al. 2001; Saulo et al. 2001).

Most of these models, evaluation has been studied under different climatic regions, namely pre-alpine region of Switzerland (Lamprecht and Berlowitz 1998), California's central valley (Hu et al. 2010), Western Australia (Hurley et al. 2001), Oresund strait, which lies between the southern part of Sweden and northern Denmark (Prabha et al. 1999), Northeastern Iberian Peninsula (NEIP) (Jiménez et al. 2006) and Southern California region (Kumar and Russell 1996). Local climatic conditions play a vital role in predicting micro meteorology and this is vindicated as we have observed distinct results from above mentioned studies. Prognostic models are observed to be sensitive to initial and boundary conditions (Kumar and Russell 1996; Prabha et al. 1999). Prabha et al. (1999) noticed that the wind speed was over predicted near the surface while simulating a mesoscale model, results showed that initialization with an early model, start time and observed wind profile near the inflow boundary improved the performance. They observed that wind speed over-prediction could be further minimized by using a more realistic objective initialization scheme. Pun et al. (2009) conducted PM simulations using Penn State University/National Center for Atmospheric Research (PSU/NCAR) Fifth Generation Mesoscale Model (MM5) (Grell et al. 1994) and the Community Multiscale Air Quality model and observed that average MM5 prognostic wind speeds were over predicted by 0.73 m s^{-1} and the average surface temperatures were over predicted by 2 K. Though MM5 has been replaced by Weather Research Forecast (WRF) (Done et al. 2004) still the majority of researchers depend on MM5 for meteorological fields for running state of art dispersion models like California Puff model (CALPUFF) (Scire et al. 2000).

The objective of this paper is to compare the surface and upper air meteorological parameters estimated from field monitoring with parameters modeled from a prognostic model. Primary parameters used for comparison are wind speed, wind direction, ambient temperature, wind speed gradient and temperature lapse rate. Derived boundary

layer parameters used for comparison are surface heat flux (H) and hourly mixing height. Sonic detection and ranging (SODAR) and Radiosonde were used for field monitoring of wind profile and temperature profile respectively in Padmapur locality near Chandrapur (India), over flat terrain. A prognostic model MM5 was modeled for Chandrapur domain and required primary meteorological parameters for comparison were extracted from it. American Meteorological Society (AMS)/Environment Protection Agency (EPA) Regulatory Model (AERMOD) (Cimorelli et al. 2005) meteorological pre-processor AERMET was used to organize and process meteorological data and to estimate the derived boundary layer parameters for comparison. Albeit, meteorological parameters can be directly compared without the use of AERMET, using AERMET enhances data quality of primary parameters and additionally derived boundary layer parameters can be estimated for comparison. As suggested by Emery et al. (2001), Hanna (1988) and Hurley et al. (2001) five simple statistical measures fractional bias (FB), mean normalized bias (MNB), correlation coefficient (R), root mean square error (RMSE) and index of agreement (IOA) were used to evaluate model output statistics.

Methodology

Field monitoring

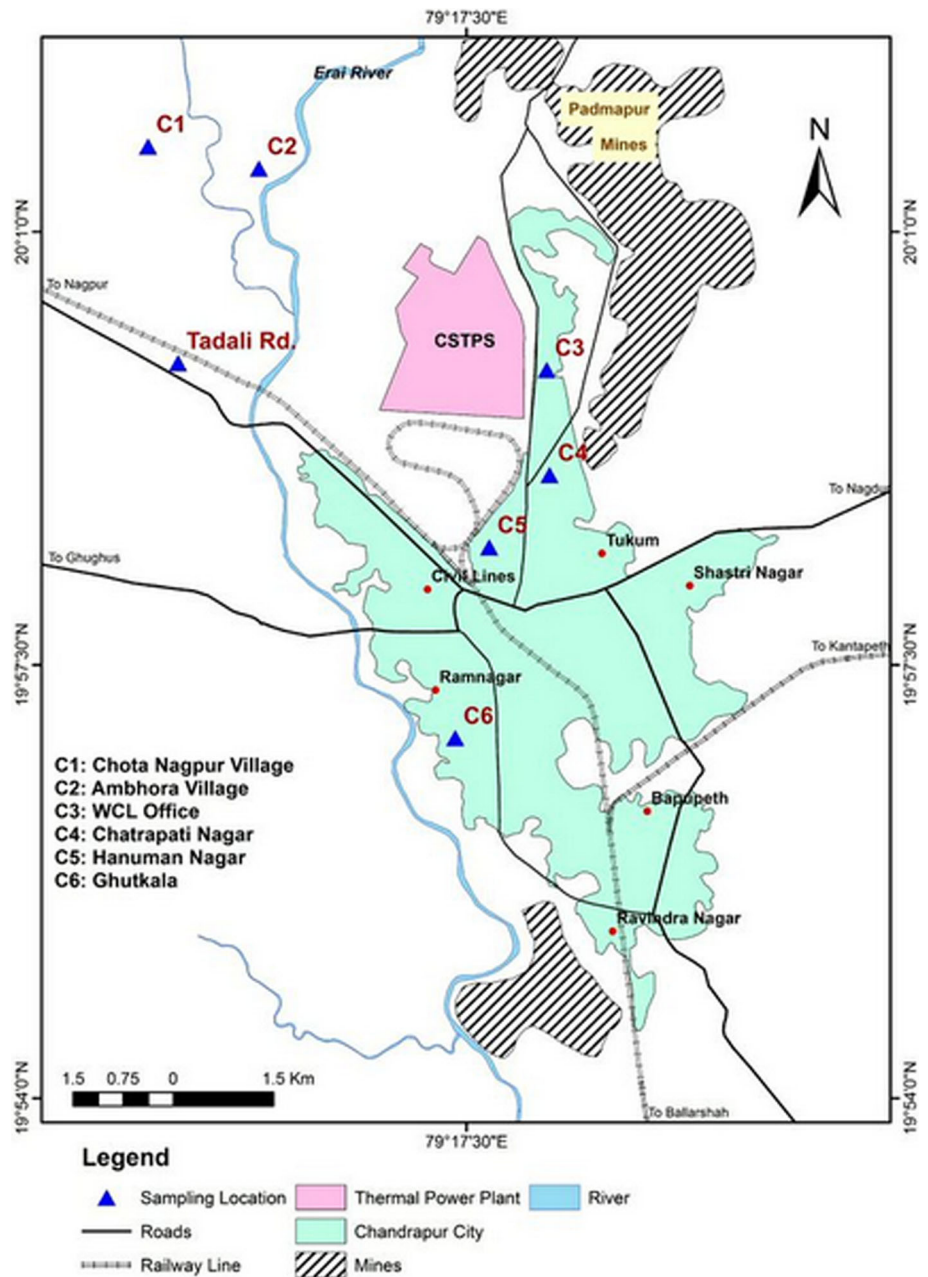
Wind profiling

A three-axis monostatic Doppler SODAR supplied by M/s. Remtech Corporation has been installed in Chandrapur, India (see Fig. 1). A Remtech PA0 phased array SODAR is a remote sensing instrument. All Remtech SODAR systems consist of one sole antenna (phased array type) and an electronic case. In the electronic case are the computer, transceiver and power amplifier. Every few second signals with five frequencies around 2250 Hz are emitted from the instrument's 196 horns which are placed on a 1.69 m^2 panel.

Information from the SODAR is averaged both in space and time. The SODAR provides a continuous record of the wind and turbulence structure of the lowest few hundred meters above ground. The instrument renders mean quantities for the echo intensity, the horizontal and vertical wind speed and the wind direction. The standard deviations of the wind measurements within every averaging period give a measure of velocity fluctuations (σ_u , σ_v , σ_w).

The Remtech SODAR is configured to record wind profiles of 44 levels between 15 and 875 m altitude every 15 min. The wind profile data quality deteriorated with increase in altitude. Possible reasons for such phenomenon

Fig. 1 Field monitoring site (C3) near Chandrapur city, India



are increased wind speeds generating ambient noise and the increased separation of air volume in relevance to the horizontal wind speed. The availability of data further depends on the ambient noise level at ground (e.g. traffic, wind).

Temperature profiling

A Mini-sonde system (model 3003 of Aero-Aqua Inc., Canada) was used for on-site measurements of the upper air temperature profile at the sampling site. The Mini-sonde system employs a small light weight sonde, which can be

used for measurement of vertical temperature profiles up to 4 km height in the atmosphere by attaching it as payload to a 15 cm balloon filled with hydrogen gas, which can lift the sand at a predetermined ascent rate (3 m s^{-1}). The Mini-sonde flight package consisting of a balloon filled with hydrogen gas, a battery operated temperature sensor and signal transmitter assembly was released to measure temperature. The temperature was measured continuously by Mini-sonde and transmitted back at 400–405 MHz frequency range to a receiving station at ground level.

The model 3003 consists an electronic modulator to process non-linearized frequency output from the receiver

into linearized signal. The modulator produces an actual temperature profile in engineering units which is fed into a plotter which produces raster images of the temperature profile.

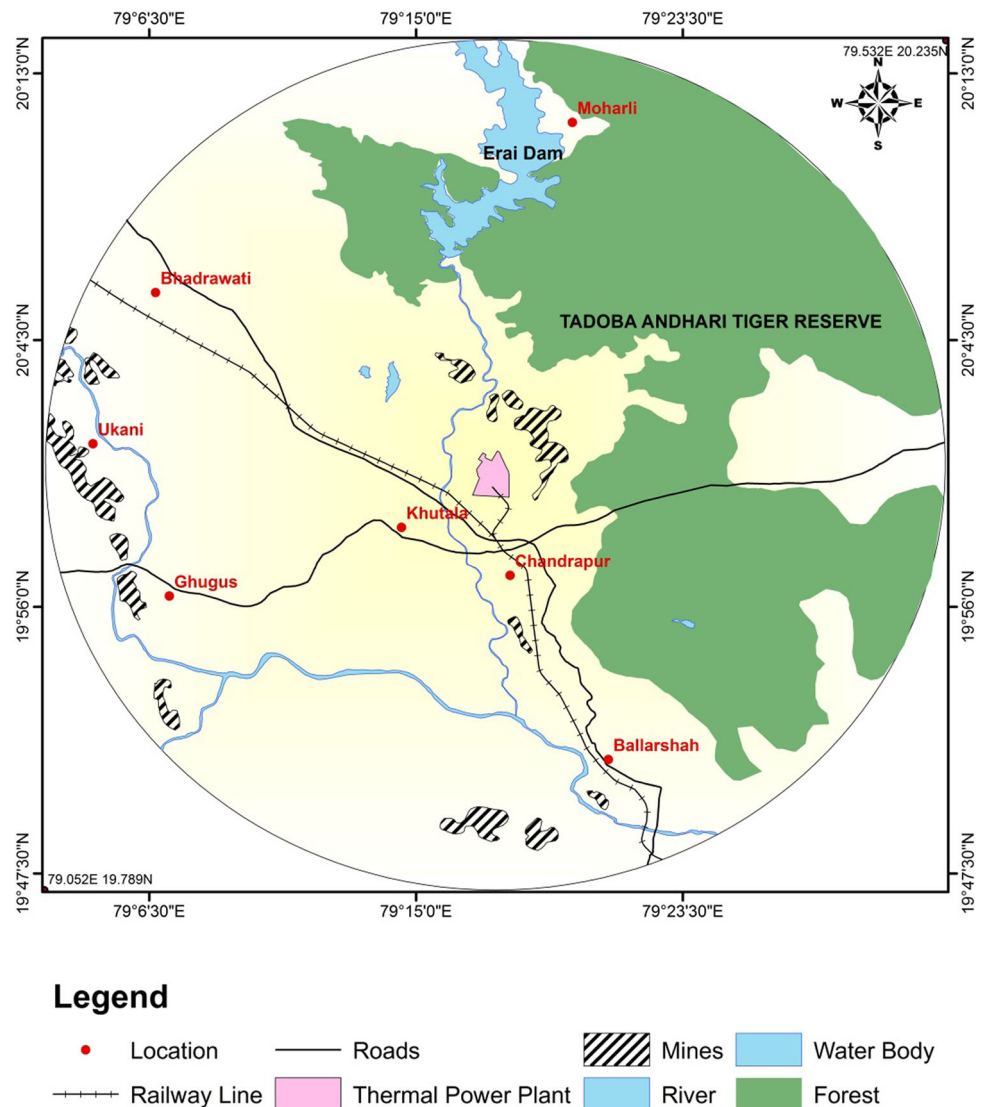
The Mini-sonde is configured to record profiles of temperature at 177 levels between 0.00096 and 1280.687 m. In the Mini-sonde, operation data were available only for the following hours: 24 UTC, 4 UTC, 7 UTC, 11 UTC, 13 UTC, 15 UTC and 16 UTC. Possible reasons for data unavailability apart from meteorological conditions are horizontal drift of balloon and the low return signal from the sensor. Therefore, analysis was carried out for above mentioned time coordinates only. The upper air temperature from Mini-sonde has been processed at levels which are similar to SODAR upper air levels. All the time coordinates mentioned here (UTC) are local Indian Standard Times.

Prognostic modeling

The primary meteorological model simulation used in this study was an annual MM5 version 3.6.1 model run, which covered the Chandrapur city (see Fig. 2) with a horizontal grid spacing of 4 km. The map projection was Lambert conformal with center latitude 19.96°N and center longitude 79.11°E. The prognostic model domain has 17 × 17 × 18 grid cells (xyz) with vertical levels reported starting from the surface at 14, 36, 109, 220, 407, 674, 990, 1357, 1783, 2229, 2696, 3189, 3980, 5155, 6510, 8119, 10,117 and 12,874 m. The model simulations were executed using the following physics options:

- Run: non hydrostatic
- Moisture options: simple ice scheme
- Cumulus parameterization: Kain–Fritsch (Kain 2004)

Fig. 2 MM5 modeled domain that was used for comparison study



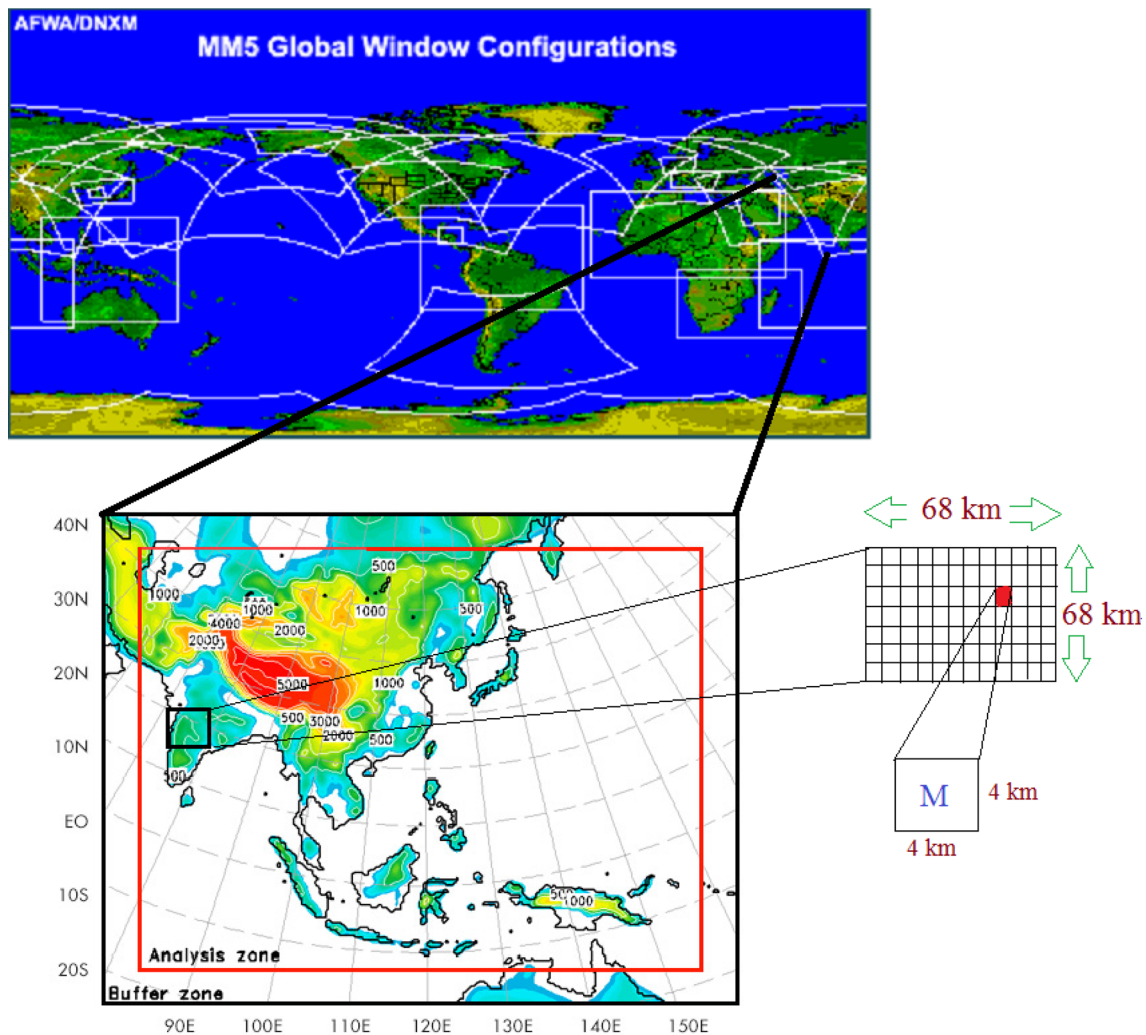


Fig. 3 Extraction of MM5 modeled data from a 4 km grid where monitoring was carried out

- PBL scheme: MRF
- Radiation scheme: cloud-radiation
- Nudging: no Four Dimensional Data Assimilation (FDDA)

Initial and boundary conditions were obtained from global forecasting model using the nesting feature of MM5.

All primary parameters of interest were extracted directly from the grid where actual monitoring was performed (see Fig. 3).

Meteorological pre-processing

Lakes Environmental AERMET View (AERMOD Meteorological Preprocessor) version 8.5.0 was used for processing meteorological data from field and model. Two sets of AERMET simulations were conducted in the current study using field monitored data and prognostic model generated data. Each of the simulations estimated primary

and derived meteorological parameters at Chandrapur, India. To run AERMET we require two input files, one surface file and one upper air file. Surface file used here is of the SAMSON format (.SAM file) and upper air file is of the TD-6201 format (.UA file).

The minimum meteorological input data required by AERMET to produce two output files (surface and profile file) are: wind speed, wind direction, ambient temperature, total sky cover or opaque sky cover (cloud cover) and morning sounding. Additional to the above parameters AERMET mandatorily requires site specific characteristics such as Bowen ratio, albedo and surface roughness length for underlying surface (AERMET user’s guide 2004).

Cloud fraction observations were assumed to be under clear sky conditions. The dew point temperature was calculated using standard formulas that are dependent on dry bulb temperature and relative humidity. For surface pressure, the pressure perturbation at the lowest model grid

level was used since this is the time varying pressure variable in the raw model output.

Cloud cover was assumed as 2 Oktas. The relative humidity around 12–20 % was assumed according to secondary data. Land use category was selected as urban and season as summer (May month in India) with Bowen ratio = 4, albedo = 0.16 and surface roughness = 1 respectively.

For the first run, input for AERMET was created using SODAR and Mini-sonde extracted data. Wind speed and wind direction were extracted from SODAR data and Temperature from Mini-sonde data. Input surface parameters for *.SAM file* were extracted from 15 m data reported by SODAR and Mini-sonde. Upper air parameters for *.UA file* were extracted from data reported by SODAR and Mini-sonde.

In the second run, input for AERMET was created using MM5 modeled surface and upper air parameters. Input surface parameters for *.SAM file* were extracted from 14 m data level as modeled by MM5. Upper air parameters for *.UA file* were extracted from all 18 sigma levels. Upper air parameters were extracted for complete 24 h as modeled by MM5. AERMET generates two output files one surface file (*.SFC*) and other profile file (*.PFL*). All required parameters for comparison, viz. Wind speed, wind direction, Temperature, sensible heat flux, mixing height and temperature lapse rate was extracted from AERMET output files. Mixing height was extracted from surface file for each case. As two mixing heights, convective and

mechanical are modeled by AERMET for each hour, the larger of convective and mechanical mixing height was chosen for day time mixing height ($L < 0$). For night time, mixing height ($L > 0$), mechanical mixing height was selected for analysis.

Results and discussion

Comparison of primary parameters (surface)

Wind speed, wind direction and temperature extracted from two AERMET output surface files (*.SFC*), one from the first run (field monitored) and another from the second run (MM5 modeled) were compared respectively.

Wind speed

MM5 modeled wind speed was compared with SODAR monitored wind speed using diurnal variation plot. Figure 4 depicts 24 h wind speed data of MM5 and SODAR processed from AERMET. Wind speeds reported from SODAR varied from 19 to 0.5 m s^{-1} with an average wind speed of 3 m s^{-1} . A large variation in wind speeds recorded by SODAR during 24 h period was observed. MM5 modeled wind speeds varied from 6.8 to 1.2 m s^{-1} with an average wind speed of 3 m s^{-1} . MM5 under predicts wind speed most of the times except for the few hours between UTC 14

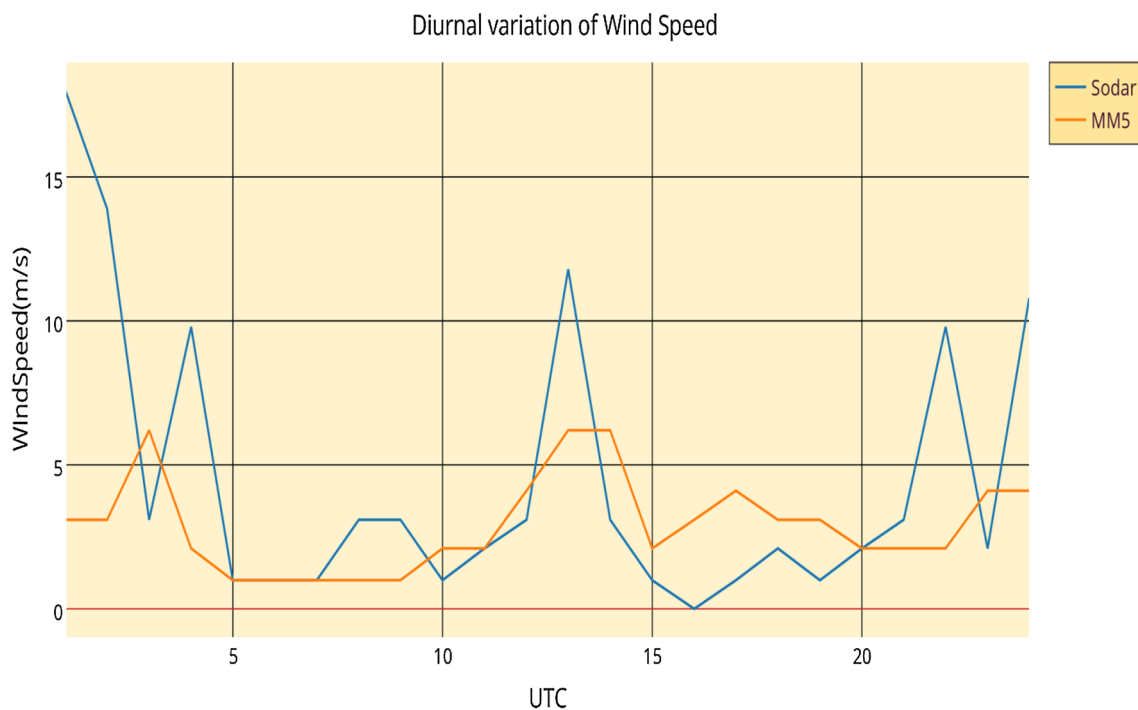


Fig. 4 Comparison of MM5 modeled and field monitored wind speed

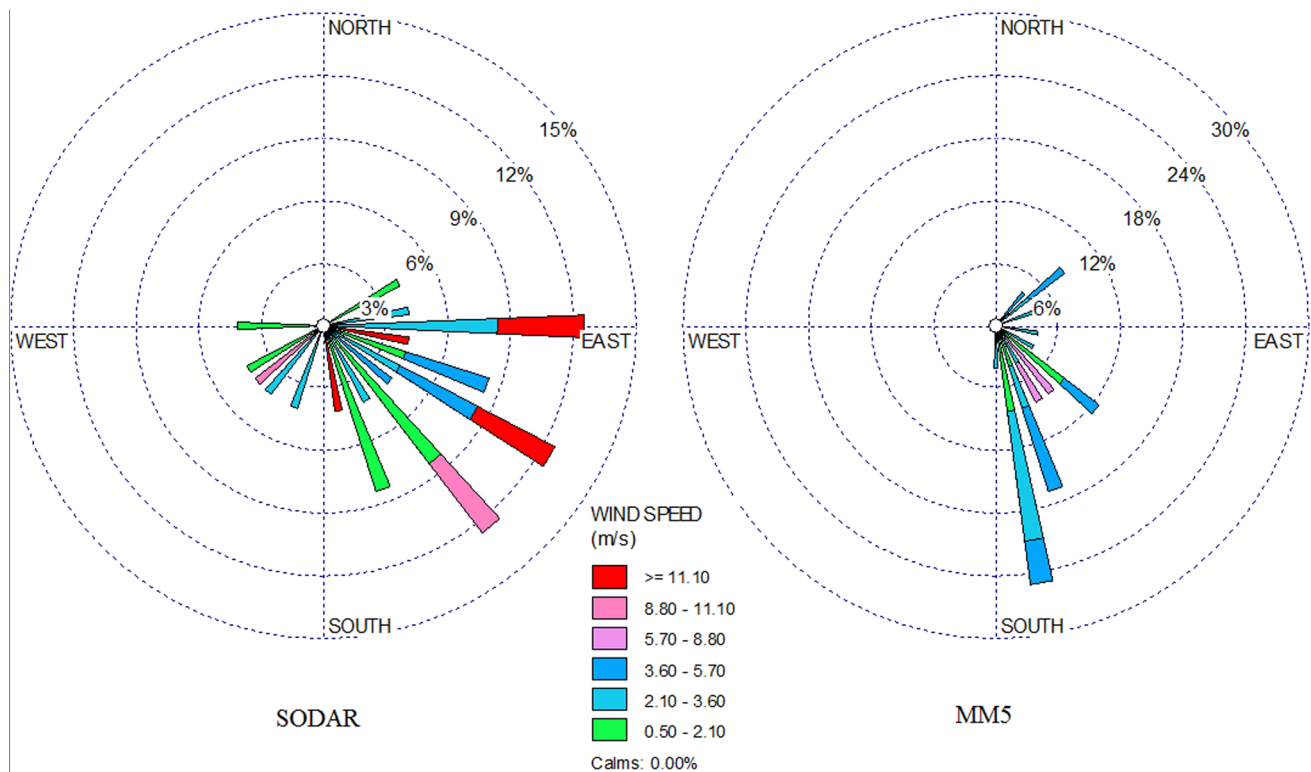


Fig. 5 Comparison of MM5 modeled and field monitored wind direction

and UTC 20. Thus, a significant difference is noticed in prediction of wind speed by prognostic model.

Wind direction

Wind rose diagram was plotted for two cases using *Lakes Environmental Wind Rose View* version 8.5.0. Figure 5 depicts wind rose diagram with the dominant wind direction and frequency of winds blowing from a particular direction over a specified period. The length of each “spoke” around the circle is related to the frequency that the wind blows from a particular direction per unit time. Each concentric circle represents a different frequency, emanating from zero at the center to increasing frequencies at the outer circles. Wind direction reported from SODAR was predominantly from southeast (SE) with large fluctuations in wind speed. MM5 modeled wind direction was predominantly from the south southeast (SSE).

Temperature

MM5 modeled temperature was compared with Mini-sonde monitored temperature using diurnal variation plot. Figure 6 depicts 24 h temperature data of MM5 and Mini-sonde processed data from AERMET. Temperatures of field monitored data varied from 46 to 34 °C with highest temperature reported at UTC 12. MM5 modeled temperature

varies from 38 to 28 °C with highest temperature reported at UTC 12. MM5 under predicts average temperature by 7 °C. The month of May in India is usually very hot and surface temperatures are recorded more than 40 °C. Thus, MM5 failed to model local meteorology.

Comparison of primary parameters (upper air)

Temperature lapse rate extracted from two AERMET output profile files (.PFL), one from the first run (field monitored) and another from the second run (MM5 modeled) were compared respectively. As AERMET processed upper air data for field monitoring was reported for 7 h, only those hours were extracted from MM5 modeled second run.

Temperature lapse rate

The increase or decrease of temperature with altitude is usually referred as lapse rate, if it represents the true atmosphere at that instant it is known as Environmental Lapse Rate (ELR) and if lapse rate is calculated assuming dry adiabatic conditions it is known as Dry Adiabatic Lapse Rate (DLR). Figure 7 compares ELR of field monitored Mini-sonde data and MM5 modeled data. Although MM5 modeled temperature data is available up to 13,000 m, only values up to 674 m were considered for

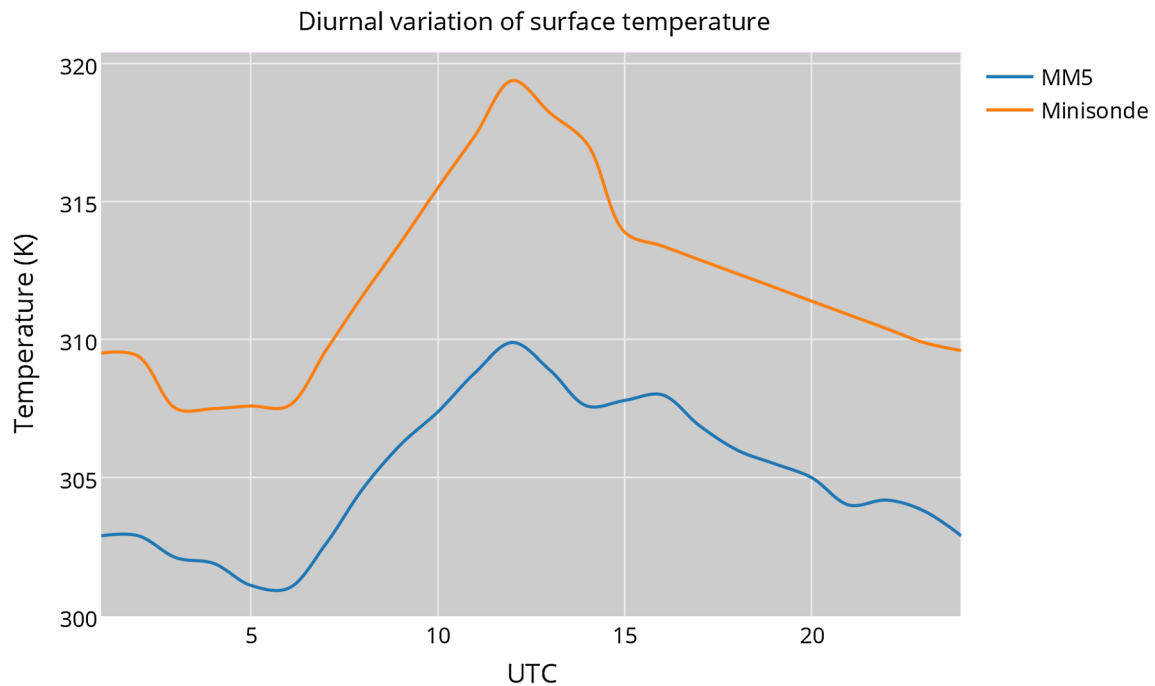


Fig. 6 Comparison of MM5 modeled and field monitored temperature

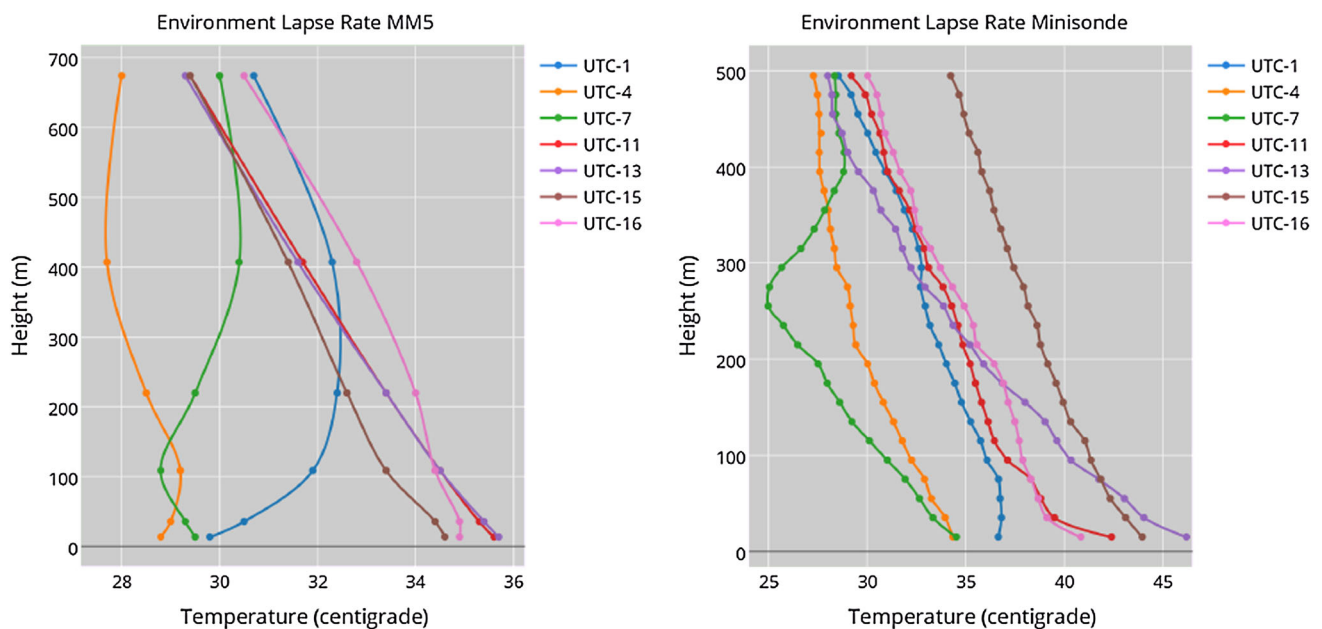


Fig. 7 Comparison of MM5 modeled and field monitored ELR

comparison. This was done because the upper air file prepared for a first AERMET run had data reported up to 500 m only. Lapse rate of only UTC 1, UTC 4, UTC 7, UTC 11, UTC 13, UTC 15 and UTC 16 were considered as Mini-sonde was monitored for these times.

ELR of MM5 modeled data at a UTC 1 depicted increase in temperature with altitude up to 300 m and then

temperature decreased with altitude. Increase in temperature with altitude leads to an inversion. When inversion occurs pollutants below the inversion height tend to stay below that level until the inversion lifts off, thereby causing severe air pollution. MM5 ELR at UTC 4 depicted inversion up to a height of 110 m. At all other times except UTC 7 temperature decreased with altitude. Field

monitored ELR at UTC 1 depicted slight inversion only up to a height of 35 m. At all other times except UTC 7 temperature decreased with altitude.

At UTC 7 ELR of modeled and monitored data depicted an elevated inversion, but at different heights. MM5 elevated inversion occurred from 100 to 400 m, whereas monitored data depicted inversion from 270 to 410 m.

Comparison of derived boundary layer parameters

Sensible heat flux and mixing height extracted from two AERMET output surface files (.SFC), one from the first run (field monitored) and another from the second run (MM5 modeled) were compared respectively.

Sensible heat flux

According to AMS, Sensible heat is somewhat archaic term that is typically the outcome of heating a surface without evaporating water from it. It is a measure of the vertical transport heat to/from the surface. Figure 8 compares the diurnal variation of sensible heat flux for two cases as mentioned above. The maximum heat flux in case of field monitored run was found to be 503.3 W m^{-2} at UTC 12 and minimum off— 3.7 W m^{-2} at UTC 22. The maximum heat flux in case of the MM5 modeled run was found to be 486.5 W m^{-2} at UTC 12 and minimum off— 64 W m^{-2} at

UTC 22. Sensible heat flux from two runs followed the same pattern of diurnal variation with MM5 modeled run under predicting sensible heat flux at each hour.

Mixing height

According to AMS, mixing height (also called mixed-layer top, mixed-layer height, and mixed-layer depth) is defined as the height at which we can locate a capping temperature inversion or statically stable layer of air and is often associated as height above which there is a sharp increase of potential temperature with height. The mixing height as defined by Seibert and Langer (1996) is the height of the layer adjacent to the ground over which pollutants or any constituents emitted within this layer or entrained in it become vertically dispersed by convection or mechanical turbulence within a time scale of about an hour.

Mixing height was compared between field monitored run and MM5 modeled run to establish the height up to which a pollutant disperses by convective as well as mechanical turbulence at each hour. It is to be noted here that field monitored run had only 7 h of upper air data as mentioned earlier, while MM5 modeled run had all 24 h upper air data.

In field monitored run as upper air data was not reported at each hour as a result the convective mixing height observed was zero for unstable conditions. Therefore, mechanical mixing height, which was observed for all

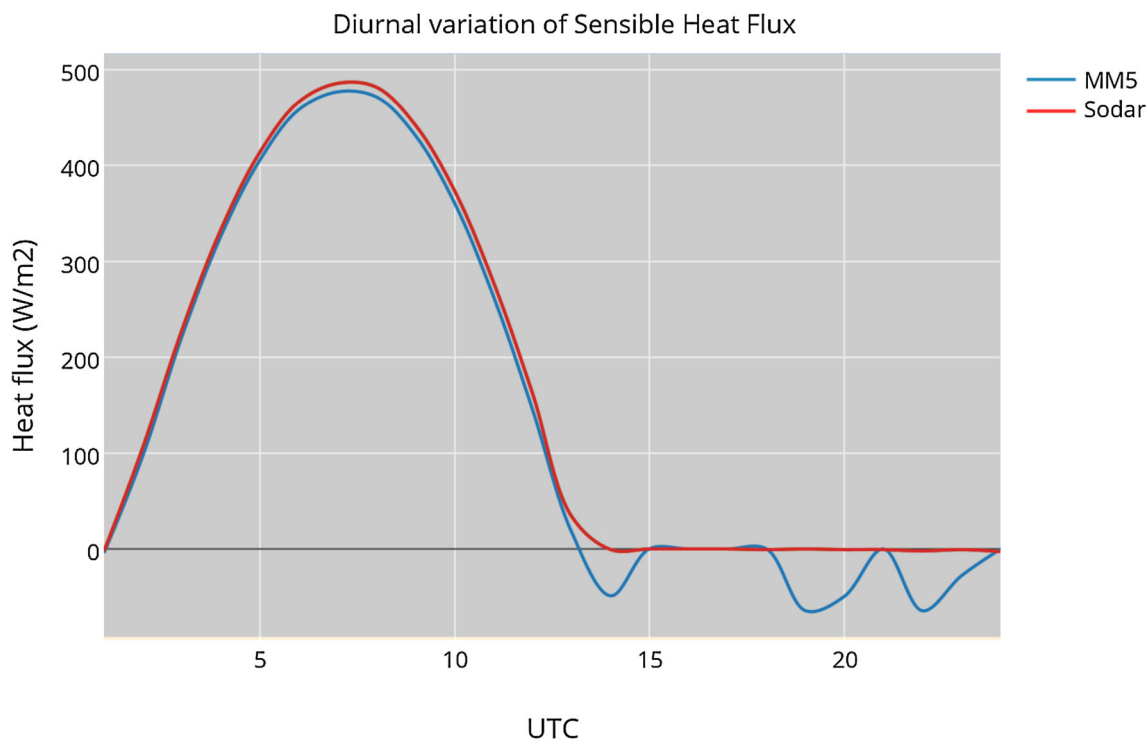


Fig. 8 Comparison of sensible heat flux estimated from MM5 modeled and field monitored AERMET run

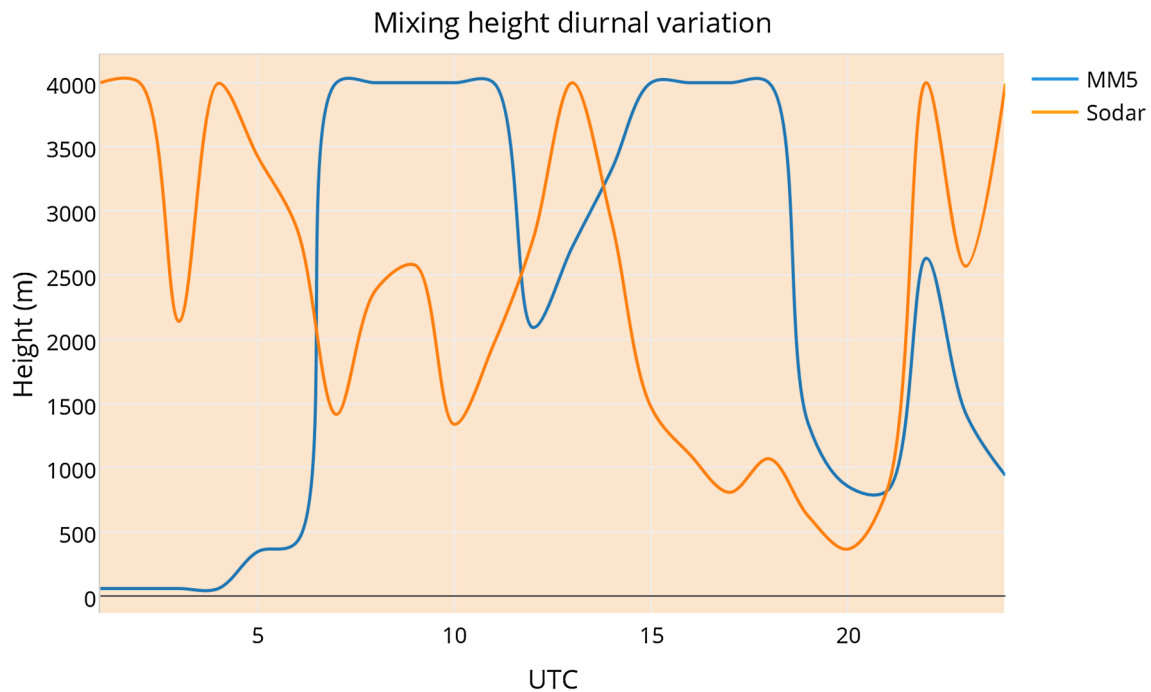


Fig. 9 Comparison of mixing height estimated from MM5 modeled and field monitored AERMET run

24 h, was used for comparison. Maximum mixing height of 4000 m was observed (see Fig. 9) at various hours as this is the maximum mixing height limit in AERMET model. Minimum mixing height of 363 m was observed at UTC 20.

MM5 modeled run showed a maximum mixing height of 4000 m at various hours during daytime. Apart from 4000 m next highest of 3320 m was found at UTC 14 and a minimum of 61 m was found at UTC 1, UTC 2, UTC 3 and UTC 4.

Mixing heights of both runs do not follow expected pattern of boundary layer evolution as mentioned by Stull (1988) but MM5 simulation closely resembles the evolution if we smoothen few hours of data. Observations here establish lack of appropriate models to predict mixing height as AERMET estimates mixing height as 4000 m for high temperatures and high wind speeds. This again shows the importance of validating models and adjusting initial and boundary conditions for different climatic conditions.

Statistical measures

Emery et al. (2001) proposed statistical benchmarks for wind speed RMSE as 2 m s^{-1} , wind speed IOA as 0.6 and temperature IOA as 0.7. Values for the FB range between -2 and $+2$ and indicate the tendency of the model to underestimate or overestimate the observed values (Lamprecht and Berlowitz 1998). Following performance statistics were calculated for analysis.

$$FB = \frac{(\bar{P} - \bar{O})}{0.5(\bar{P} + \bar{O})}$$

$$MNB = \frac{1}{N} \sum_{i=1}^N \left(\frac{P_i - O_i}{O_i} \right)$$

$$R = \frac{\frac{1}{N} \sum_{i=1}^N (O_i - \bar{O})(P_i - \bar{P})}{\sigma_P \sigma_O}$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (P_i - O_i)^2}$$

$$IOA = 1 - \frac{\sum_{i=1}^N (P_i - O_i)^2}{\sum_{i=1}^N (|P_i - \bar{P}| + |O_i - \bar{O}|)^2}$$

where, \bar{P} and \bar{O} denote the mean predicted and observed parameters, respectively. P_i and O_i denote the individual predicted and observed parameters each hour, respectively. σ_P and σ_O denote the standard deviation of predicted and observed parameters each hour, respectively.

Table 1 shows the results of the performance measures FB, IOA, MNB, R, RMSE and their ideal values. Means of observed and predicted meteorological parameters for an ensemble of 24 h data are also tabulated. MNB values close to zero are ideal for accuracy of prediction, only temperature with -0.02 MNB was close to zero. FB values show under prediction and over prediction by a model with values close to 0 as ideal. FB values for temperature, H and mixing height were close to zero indicating satisfactory

Table 1 Statistical measures for evaluating performance of a prognostic model in predicting meteorological parameters

Statistics	Wind speed (m s ⁻¹)	Temperature (K)	H (W m ⁻²)	Mixing height (m)	Ideal
IOA	0.12	-0.39	0.99	0.21	1.00
MNB	0.44	-0.02	38.4	0.50	0.00
R	-0.25	0.92	0.95	-0.39	1.00
RMSE	5.70	7.02	23.2	2397.2	0.00
FB	-0.11	-0.00	-0.02	-0.015	0.00
\bar{O}	4.50	312	159.9	2358.3	-
\bar{P}	2.92	305	145.5	2214.6	-

performance. RMSE values close to 0 are considered ideal, but all the values evaluated show very high RMSE indicating poor performance of the model. R close to 1 is considered ideal with the value 1 indicating good positive correlation. Temperature and Sensible heat flux with R values as 0.92 and 0.95 indicate very good relation between model and observed values. Index of Agreement values close to 1 are ideal case, but values >0.5 are considered to be good for meteorological data. Surface Heat Flux with IOA value of 0.99 indicates excellent agreement with modeled value with the remaining parameters showing very weak agreement with modeled data. Overall Temperature and Sensible heat flux showed good correlation even though the temperature was under predicted by MM5 simulation. It is to be noted that these measures are very sensitive to outliers therefore more robust simulation may be performed for accurate statistical measures of all parameters.

Conclusion

In this study, a meteorological preprocessing model (AER-MET) was used for comparing prognostic model generated meteorological parameters with field monitored meteorological parameters over flat terrain at Padmapur locality near Chandrapur, India. Comparison of the predicted and measured meteorological time series shows that the MM5 prognostic model does not accurately simulate meteorological temperature and wind fields. Wind direction of the model was predominantly from SSE whereas field monitored wind direction was from the SE. Wind speed observed from SODAR was higher than the model predicted value. Temperature data from the Mini-sound was compared to MM5 modeled data and it was observed that MM5 under predicted temperature by 7 °C. Although MM5 under predicted sensible heat flux it captured overall diurnal variation of heat flux. Statistical measures were calculated to evaluate model performance. FB values for temperature, H and mixing height are close to zero indicating satisfactory performance. Very high RMSE indicated poor performance of primary parameters. Temperature and Sensible heat flux with R values as 0.92 and 0.95 indicate very good

relation between model and observed values. Surface Heat Flux with IOA value of 0.99 indicates excellent agreement with modeled value.

The results indicate that use of prognostic modeled meteorological parameters did not give satisfactory results. There is need to recalibrate such prognostic models for different climatic conditions. Terrain and Land use data must be accurately used in the model for better accuracy. To arrive at some definite conclusions further research with data nudging and new statistical measures may be studied. In case of statistical measures a definite benchmark is to be established. The prognostic models are being increasingly used in air quality modeling studies, especially when there is a lack of measured data to use a diagnostic model. Most often these measurements are not available and prognostic models are the only models that can be used to develop meteorological data in those cases. Thus, there is a need to further develop the prognostic models and further investigate their effect on air quality model results and control strategy evaluations. Until then, one should consider alternative wind fields, and objectively compare the input fields for their representativeness. The downscaling of model domain needs to be analyzed for a better input of initial and boundary conditions.

Compliance with ethical standards

Conflict of interest The authors declare that they have no conflict of interest.

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