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## **MCL732 ASSIGNMENT-4 REPORT**

### **Performance of WRF/Chem over Bihar, Jharkhand, and West Bengal**

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#### **1. Introduction**

This report evaluates the performance of the Weather Research and Forecasting model coupled with Chemistry (WRF/Chem) over the regions of Bihar, Jharkhand, and West Bengal. The primary objective is to compare simulated gas-phase pollutants and particulate matter (PM10 and PM2.5) concentrations with real-world data from Central Pollution Control Board (CPCB) stations.

## 2. Background

### 2.1. WRF/Chem Model Overview

WRF/Chem is a regional atmospheric model that incorporates chemical transport, emission, deposition, and photochemical reactions. It allows for the simulation of air quality, providing insights into pollutant dispersion and chemical transformation.

### 2.2. Importance of Model Evaluation

Model validation using observational data is crucial for ensuring its reliability. By comparing simulations with CPCB data, this study assesses the model's accuracy in capturing pollutant concentrations.

## 3. Methodology

### 3.1. Study Region

The study focuses on **Bihar, Jharkhand, and West Bengal**, which experience frequent air pollution episodes due to industrial activities, vehicular emissions, and biomass burning.

### 3.2. Pollutants Considered

- Gas-Phase Pollutants: NO, NO<sub>2</sub>, O<sub>3</sub>, SO<sub>2</sub>, CO, NH<sub>3</sub>
- Particulate Matter: PM<sub>10</sub> and PM<sub>2.5</sub>

### 3.3. Grid Resolution

The simulations were conducted at a horizontal grid resolution of 50 km x 50 km, ensuring computational efficiency while capturing regional pollution dynamics.

### 3.4. Temporal Resolution

Hourly data were extracted for comparison with CPCB stations.

## 4. Model Setup and Configuration

### 4.1. Domain Configuration

- Domain: Bihar, Jharkhand, and West Bengal
- Resolution: 20 km x 20 km
- Vertical Levels: 45

- Time Step: 60 seconds

```

wrffirechemi_d01_2021-01-01_15:00:00 wrffirechemi_d01_2021-01-13_00:00:00 wrfrst_d01_2021-01-16_00:00:00
wrffirechemi_d01_2021-01-01_16:00:00 wrffirechemi_d01_2021-01-13_01:00:00 wrfrst_d01_2021-01-16_00:00:00
wrffirechemi_d01_2021-01-01_17:00:00 wrffirechemi_d01_2021-01-13_02:00:00 wrfrst_d01_2021-01-16_00:00:00
wrffirechemi_d01_2021-01-01_18:00:00 wrffirechemi_d01_2021-01-13_03:00:00 wrfrst_d01_2021-01-16_00:00:00
wrffirechemi_d01_2021-01-01_19:00:00 wrffirechemi_d01_2021-01-13_04:00:00 wrfrst_d01_2021-01-16_00:00:00
wrffirechemi_d01_2021-01-01_20:00:00 wrffirechemi_d01_2021-01-13_05:00:00 wrfrst_d01_2021-01-16_00:00:00
wrffirechemi_d01_2021-01-01_21:00:00 wrffirechemi_d01_2021-01-13_06:00:00 wrfrst_d01_2021-01-16_00:00:00
wrffirechemi_d01_2021-01-01_22:00:00 wrffirechemi_d01_2021-01-13_07:00:00 wrfrst_d01_2021-01-16_00:00:00
wrffirechemi_d01_2021-01-01_23:00:00 wrffirechemi_d01_2021-01-13_08:00:00 wrfrst_d01_2021-01-16_00:00:00
wrffirechemi_d01_2021-01-02_00:00:00 wrffirechemi_d01_2021-01-13_09:00:00 wrfrst_d01_2021-01-16_00:00:00
wrffirechemi_d01_2021-01-02_01:00:00 wrffirechemi_d01_2021-01-13_10:00:00 wrfrst_d01_2021-01-16_00:00:00
wrffirechemi_d01_2021-01-02_02:00:00 wrffirechemi_d01_2021-01-13_11:00:00 wrfrst_d01_2021-01-16_00:00:00
wrffirechemi_d01_2021-01-02_03:00:00 wrffirechemi_d01_2021-01-13_12:00:00 wrfrst_d01_2021-01-16_00:00:00
wrffirechemi_d01_2021-01-02_04:00:00 wrffirechemi_d01_2021-01-13_13:00:00 wrfrst_d01_2021-01-16_00:00:00
wrffirechemi_d01_2021-01-02_05:00:00 wrffirechemi_d01_2021-01-13_14:00:00 wrfrst_d01_2021-01-16_00:00:00
wrffirechemi_d01_2021-01-13_15:00:00 wrfrst_d01_2021-01-16_00:00:00 wrf_season_wes_usgs_d01.nc

[vst249006@login04 ~/scratch/WRF-release-v4.2.2/test/em_real]
$ tail -f rsl.error.0000
DEBUG output wrf(): before call to domain_clock_get, clock current time = 2021-01-20 00:00:00
DEBUG output wrf(): before call to domain_clock_get, clock stop time = 2021-01-20 00:00:00
DEBUG output wrf(): before call to domain_clock_get, clock time step = 0000000000 000:00:030
d01 2021-01-20 00:00:00 DEBUG wrf_timetoea(): returning with str = [2021-01-20 00:00:00]
d01 2021-01-20 00:00:00 med_hist_out: opened wrfout_d01_2021-01-20_00:00:00 as DATASET=HISTORY
Timing for Writing wrfout_d01_2021-01-20_00:00:00 for domain 1: 5.31972 elapsed seconds
d01 2021-01-20 00:00:00 wrf: back from integrate
d01 2021-01-20 00:00:00 Entering ext_gr1_ioexit
d01 2021-01-20 00:00:00 wrf: back from med shutdown to
d01 2021-01-20 00:00:00 wrf: SUCCESS COMPLETE WRF

```

Fig.WRF Built Result

## 4.2. Chemical Mechanism

The CBMZ (Carbon Bond Mechanism Z) was applied for gas-phase chemistry, while the MOSAIC (Model for Simulating Aerosol Interactions and Chemistry) scheme was used for aerosol representation.

### PYTHON CODE:

```
import xarray as xr
```

```
import numpy as np
```

```
import pandas as pd
```

```
import os
```

```
# Directory containing the files
```

```
data_dir = "/home/visitor/student/vst249006/scratch/WRF-release-  
v4.2.2/test/em_real/Ayaanres/"
```

```
# Get all .nc files (sorted by date)
```

```
file_names = sorted([f for f in os.listdir(data_dir) if f.startswith("wrfout_d01_2021-01") and  
f.endswith(".nc")])
```

```
# Define pollutants
```

```
pollutants = ["PM2_5_DRY", "PM10", "o3", "no", "no2", "so2", "co", "nh3"]
```

```
# Conversion factors (ppb →  $\mu\text{g}/\text{m}^3$  at 25°C, 1 atm)
```

```
conversion_factors = {"o3": 1.96, "no": 1.23, "no2": 1.88, "so2": 2.62, "co": 1.15, "nh3":  
0.77}
```

```
# Target location
```

```
target_lat = 25.6059
```

```
target_lon = 85.1097
```

```
# Store extracted data
```

```
data_list = []
```

```
# Loop through each file
```

```
for file in file_names:
```

```
    file_path = os.path.join(data_dir, file)
```

```
    date_str = file.split("_")[-1].split(".nc")[0] # Extract date
```

```
    date = pd.to_datetime(date_str)
```

```

# Include up to Jan 20th at 00:00:00

if date > pd.to_datetime("2021-01-20 00:00:00"):

    break


# Load dataset

ds = xr.open_dataset(file_path)


# Find nearest grid point to target lat/lon

latitudes = ds["XLAT"].isel(Time=0).values

longitudes = ds["XLONG"].isel(Time=0).values


lat_idx, lon_idx = np.unravel_index(((latitudes - target_lat)**2 + (longitudes -
target_lon)**2).argmin(), latitudes.shape)


# Extract hourly data

for t in range(ds.dims["Time"]):

    time_bytes = ds["Times"].isel(Time=t).values.tobytes().decode('utf-8')

    time_str = pd.to_datetime(time_bytes, format='%Y-%m-%d_%H:%M:%S')

    values = {"DateTime": time_str}


    for pollutant in pollutants:

        if pollutant in ds.variables:

            conc = ds[pollutant].isel(Time=t, bottom_top=0, south_north=lat_idx,
west_east=lon_idx).values


            if pollutant in conversion_factors:

                conc *= conversion_factors[pollutant] # Convert to µg/m³

```

```
values[pollutant] = conc
```

```
data_list.append(values)
```

```
ds.close()
```

```
# Convert to DataFrame
```

```
df = pd.DataFrame(data_list)
```

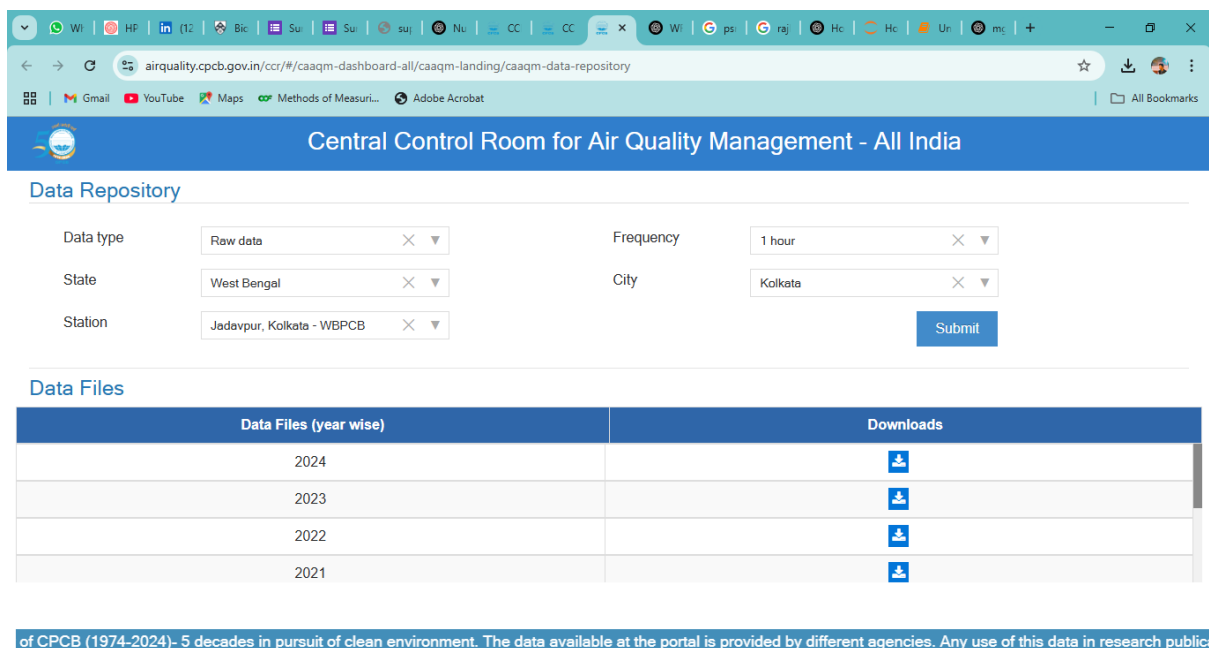
```
df.to_csv("hourly_pollutant_concentration.csv", index=False)
```

```
print("Data saved to hourly_pollutant_concentration.csv")
```





## 5. Data Collection and Processing

### 5.1. CPCB Data

Hourly and daily concentration data from CPCB monitoring stations were obtained for comparison.



The screenshot displays the 'Data Repository' page of the Central Control Room for Air Quality Management - All India. The page features a search form with the following fields: Data type (Raw data), Frequency (1 hour), State (West Bengal), City (Kolkata), and Station (Jadavpur, Kolkata - WBPCB). A 'Submit' button is located to the right of the search form. Below the search form, there is a section titled 'Data Files' which contains a table with two columns: 'Data Files (year wise)' and 'Downloads'. The table lists data files for the years 2024, 2023, 2022, and 2021, each with a corresponding download icon.

Data Files (year wise)	Downloads
2024	
2023	
2022	
2021	

of CPCB (1974-2024)- 5 decades in pursuit of clean environment. The data available at the portal is provided by different agencies. Any use of this data in research publica

### 5.2. Data Extraction from WRF Output

NetCDF files were processed using Python to extract pollutant concentrations at the corresponding CPCB station locations.

### 5.3. Spatial Averaging

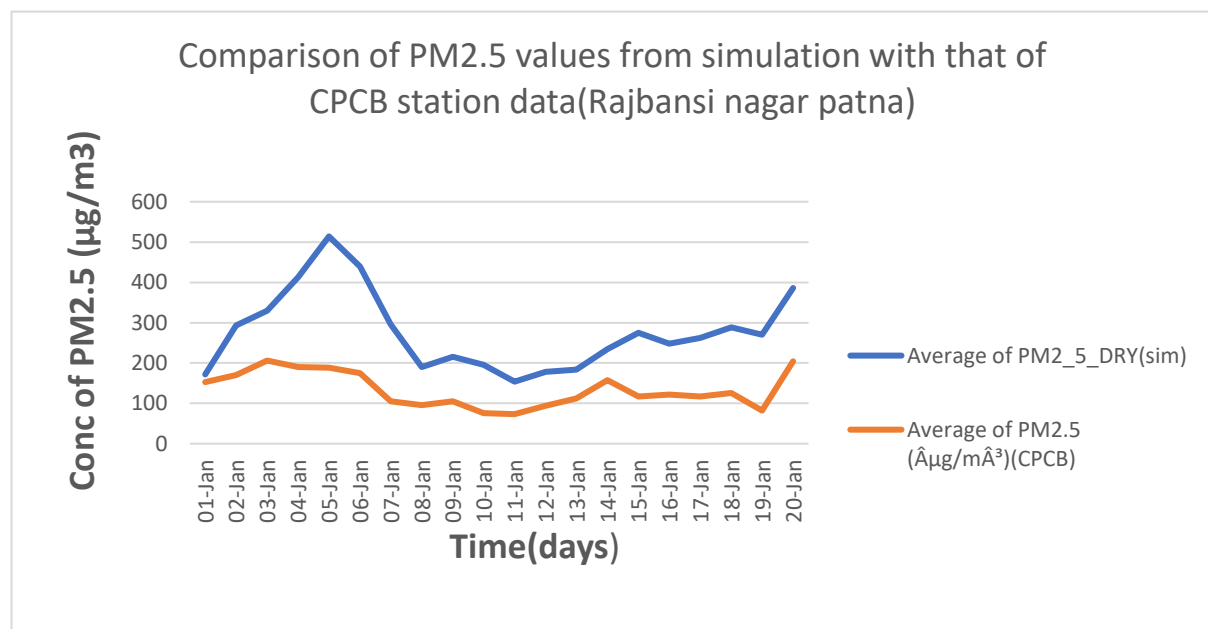
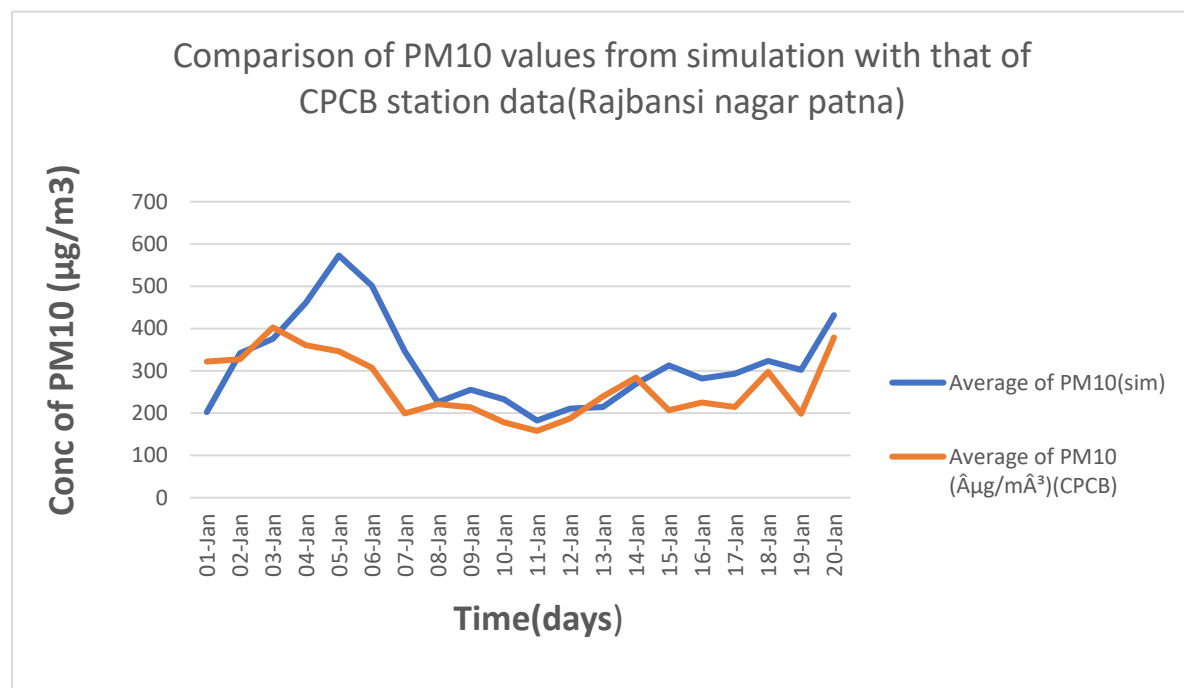
- If one CPCB station fell within a grid, its data were used.
- If multiple stations were within a single grid, the values were averaged.

## 6.Results

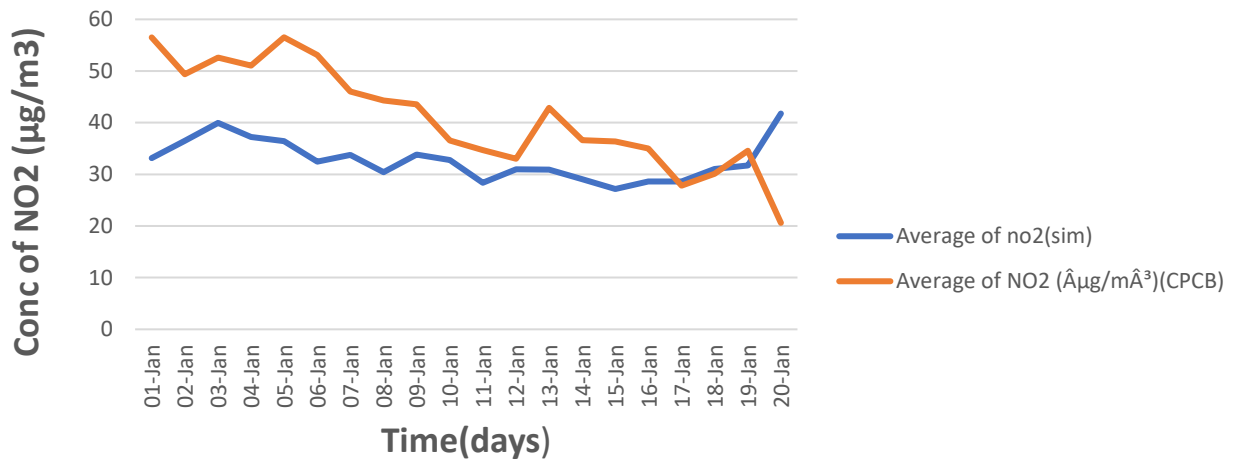
### DAILY VARIATION TIME SERIES:

a)State:BIHAR

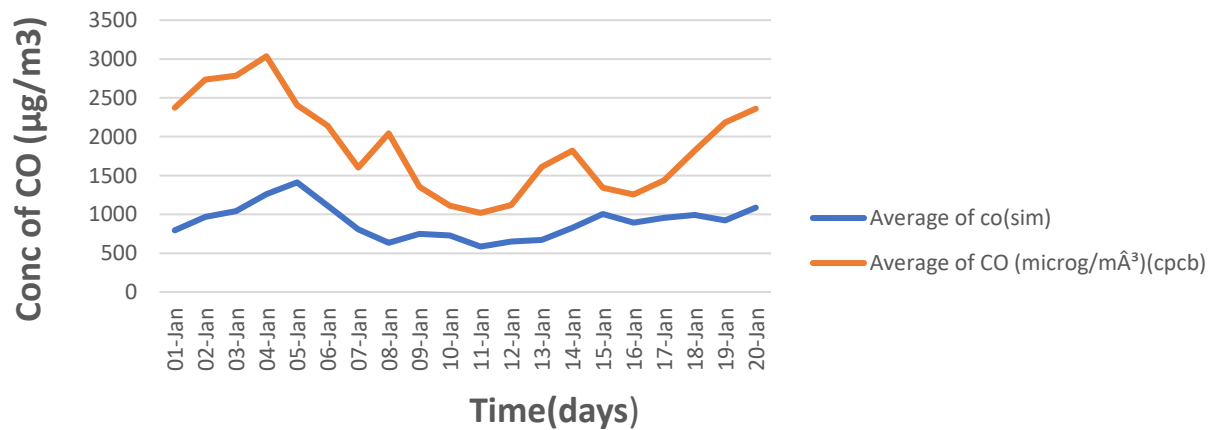
Monitoring Station:RAJBANSI NAGAR PATNA STATION



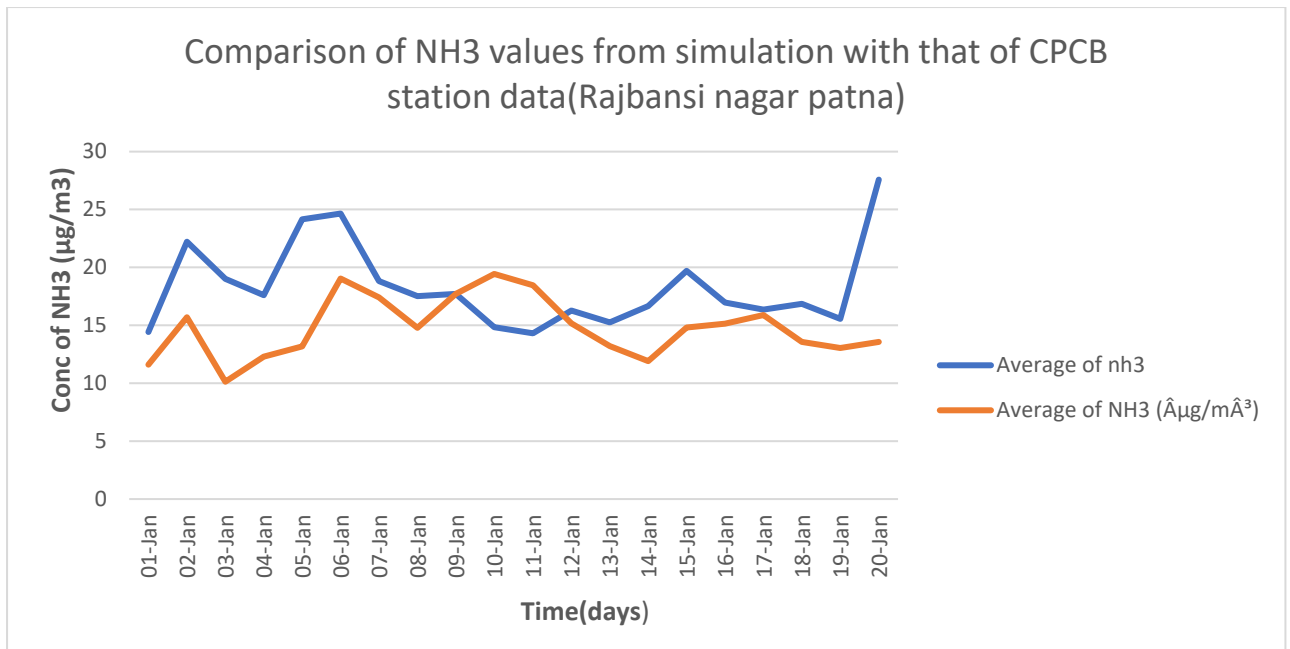
Comparison of NO<sub>2</sub> values from simulation with that of CPCB station data(Rajbansi nagar patna)



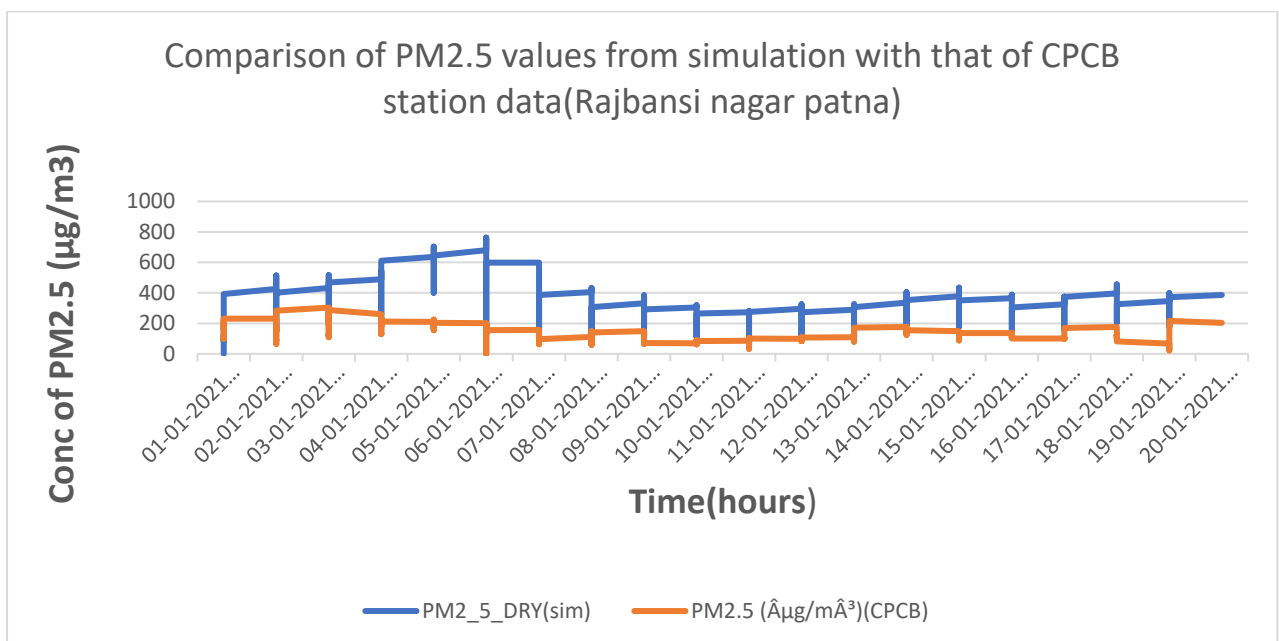
Comparison of CO values from simulation with that of CPCB station data(Rajbansi nagar patna)

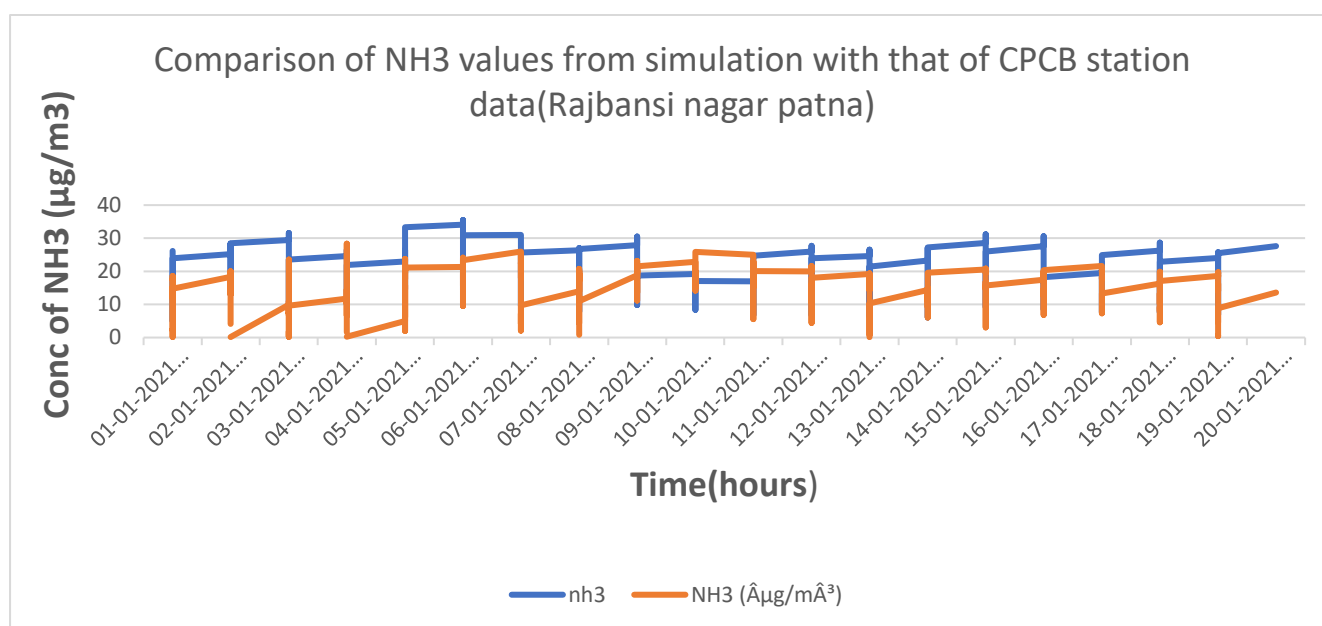
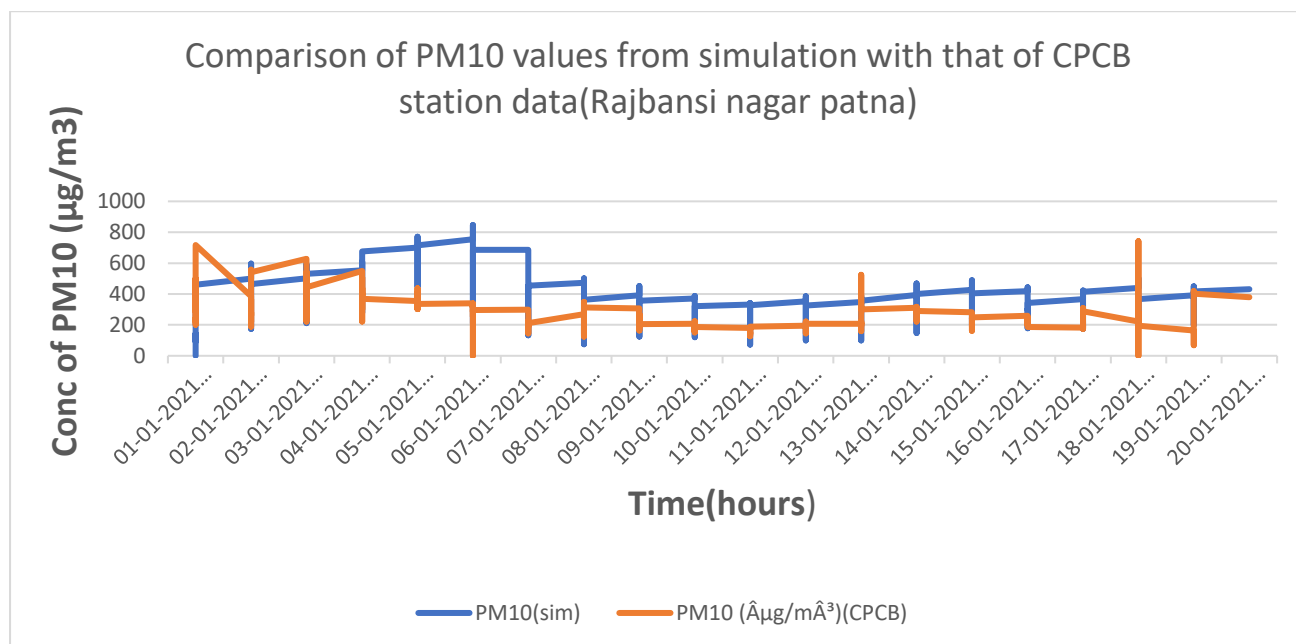


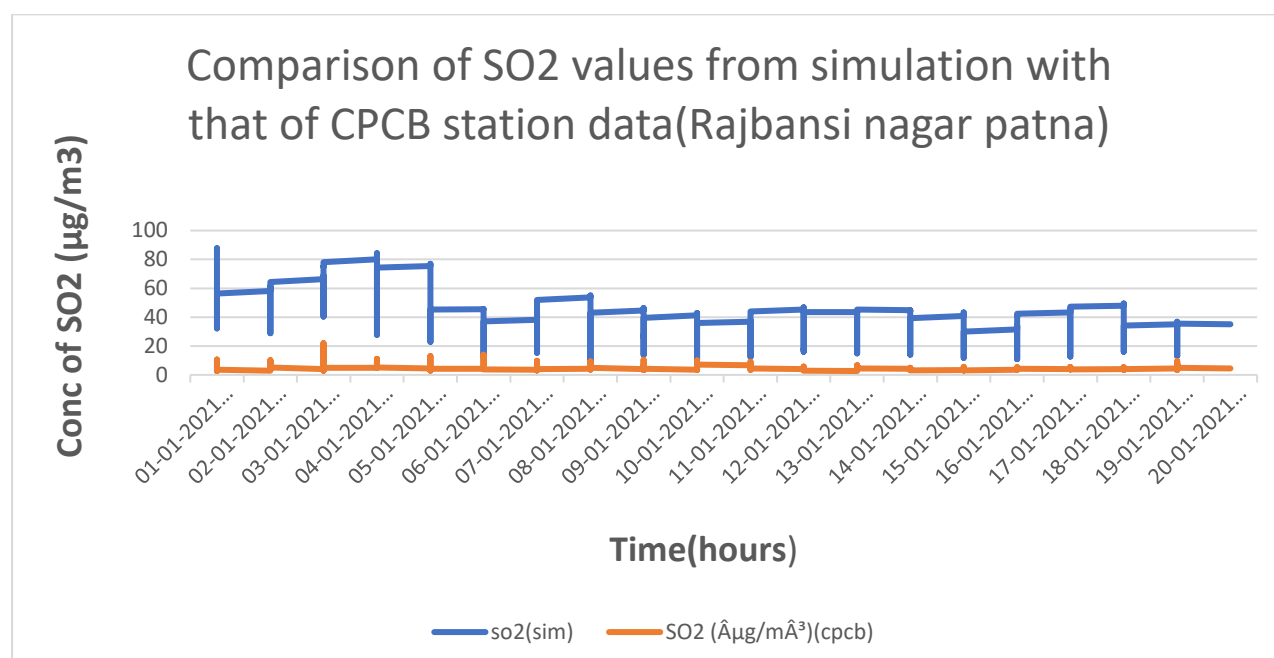
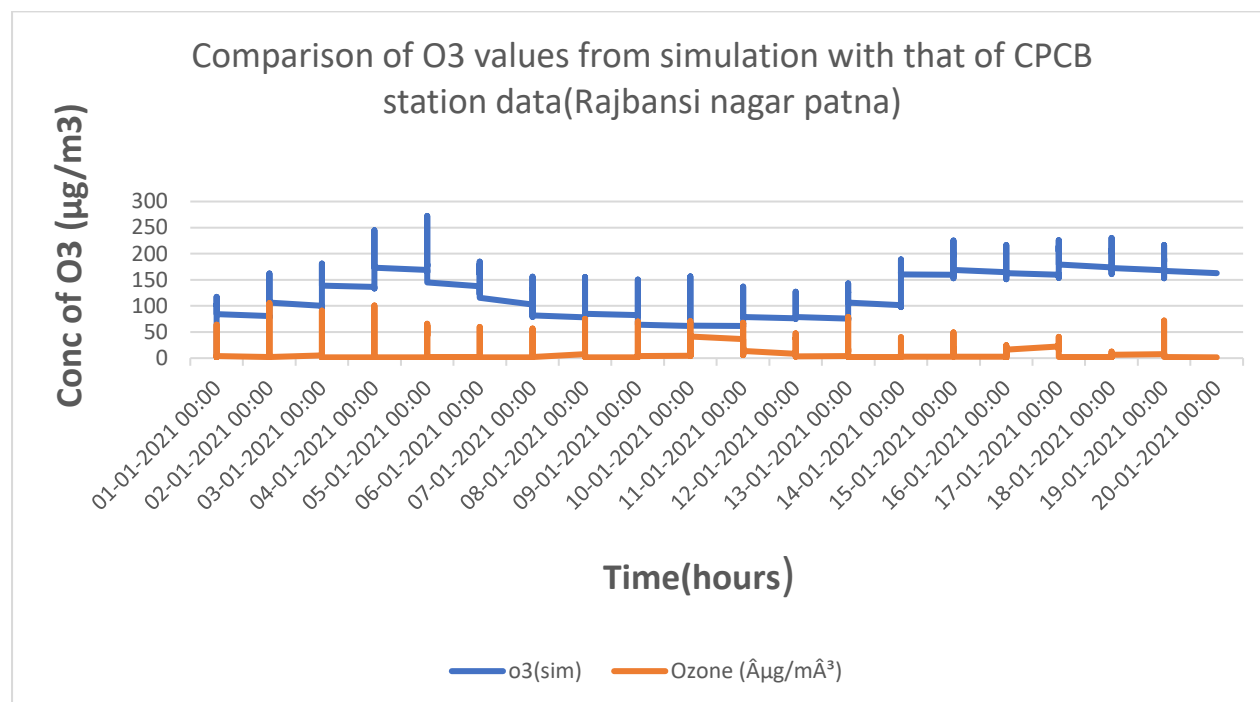




### DIURNAL VARIATION TIME SERIES:



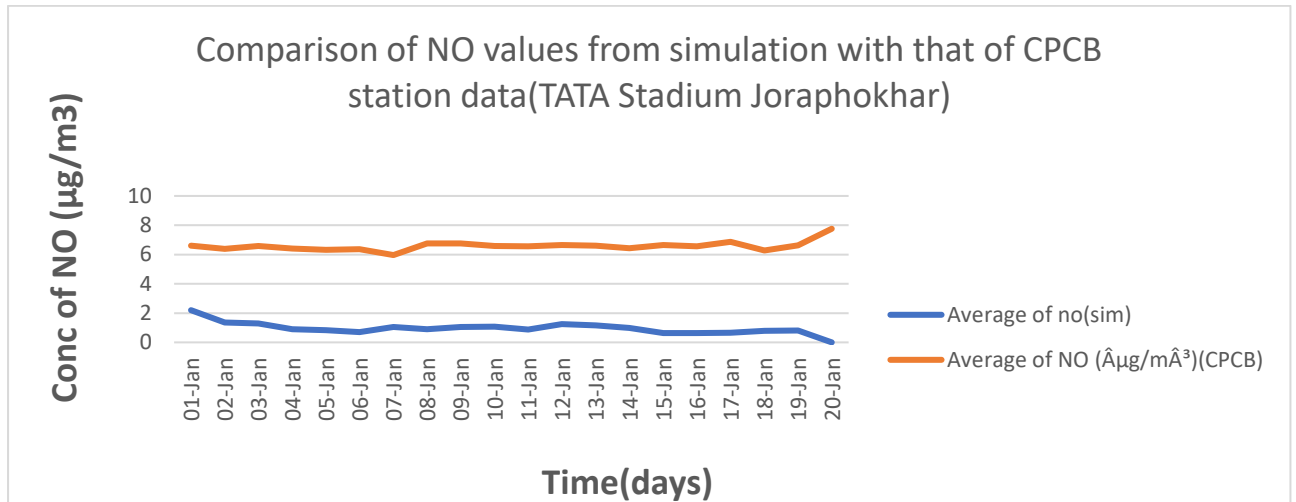




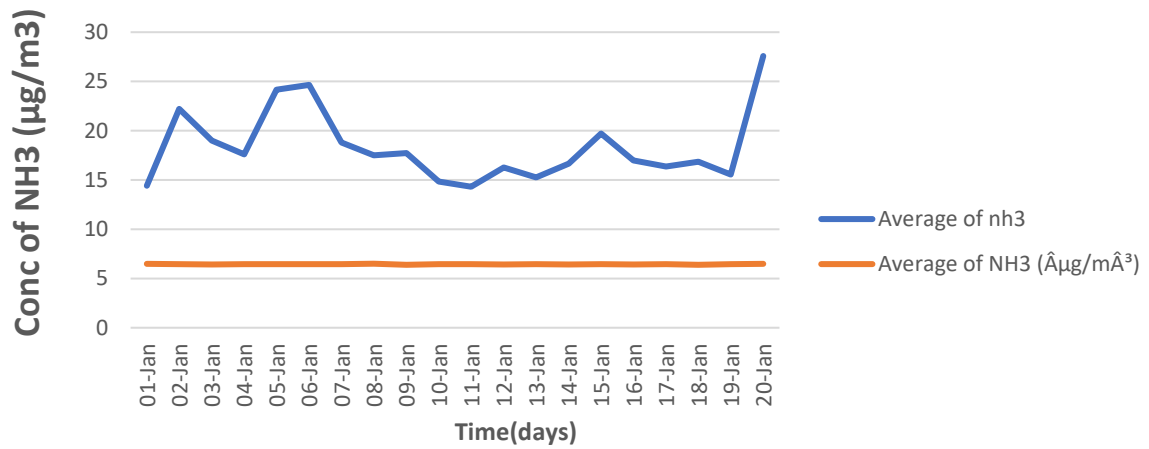
## **DAILY VARIATION TIME SERIES:**

**b)State:Jharkhand**

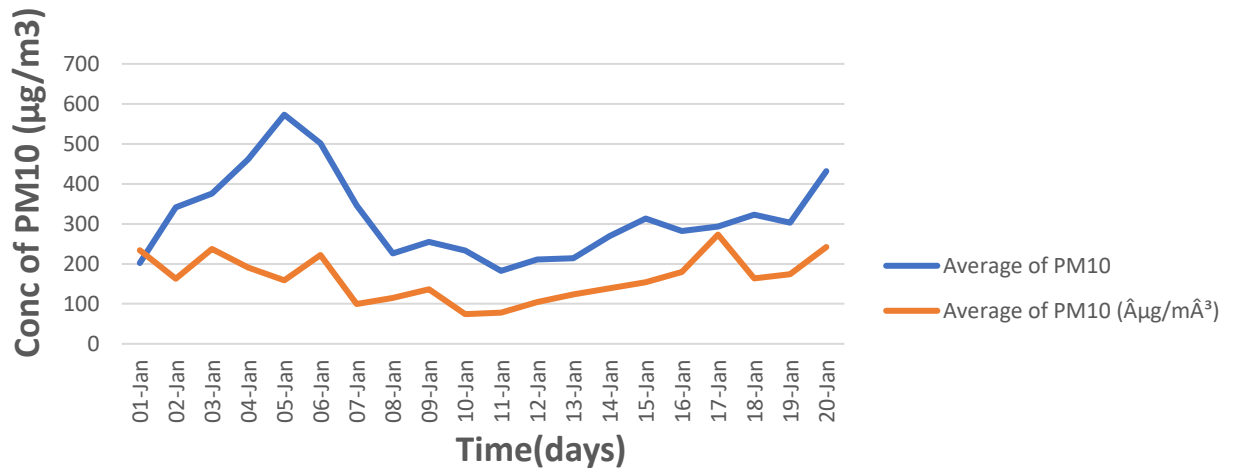
**Monitoring station:TATA STADIUM JORAPHOKHAR**

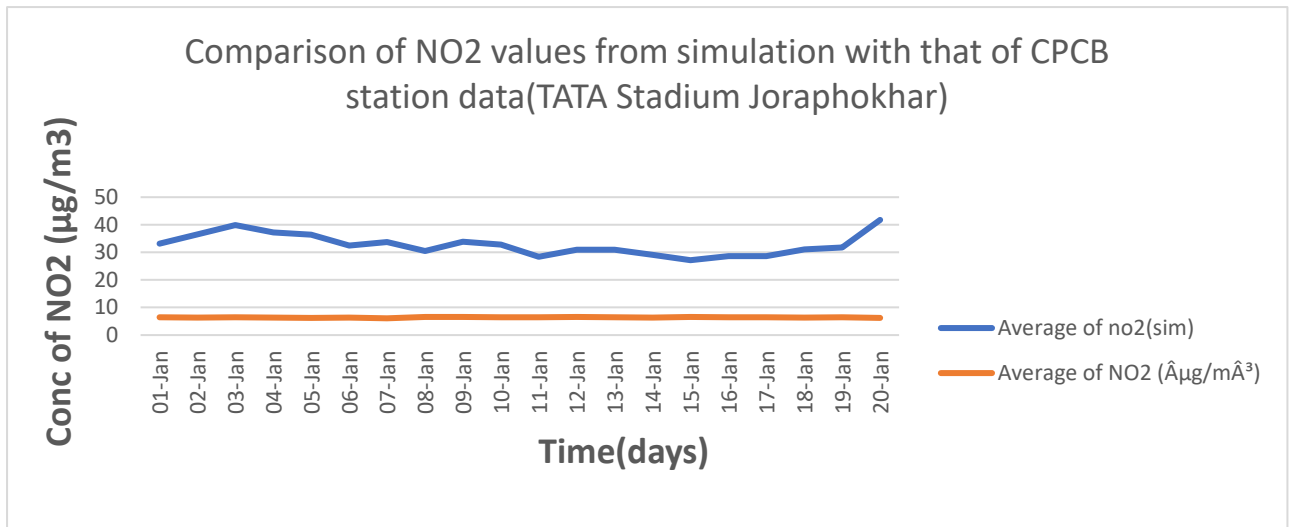


Comparison of NH<sub>3</sub> values from simulation with that of CPCB station data(TATA Stadium Joraphokhar)

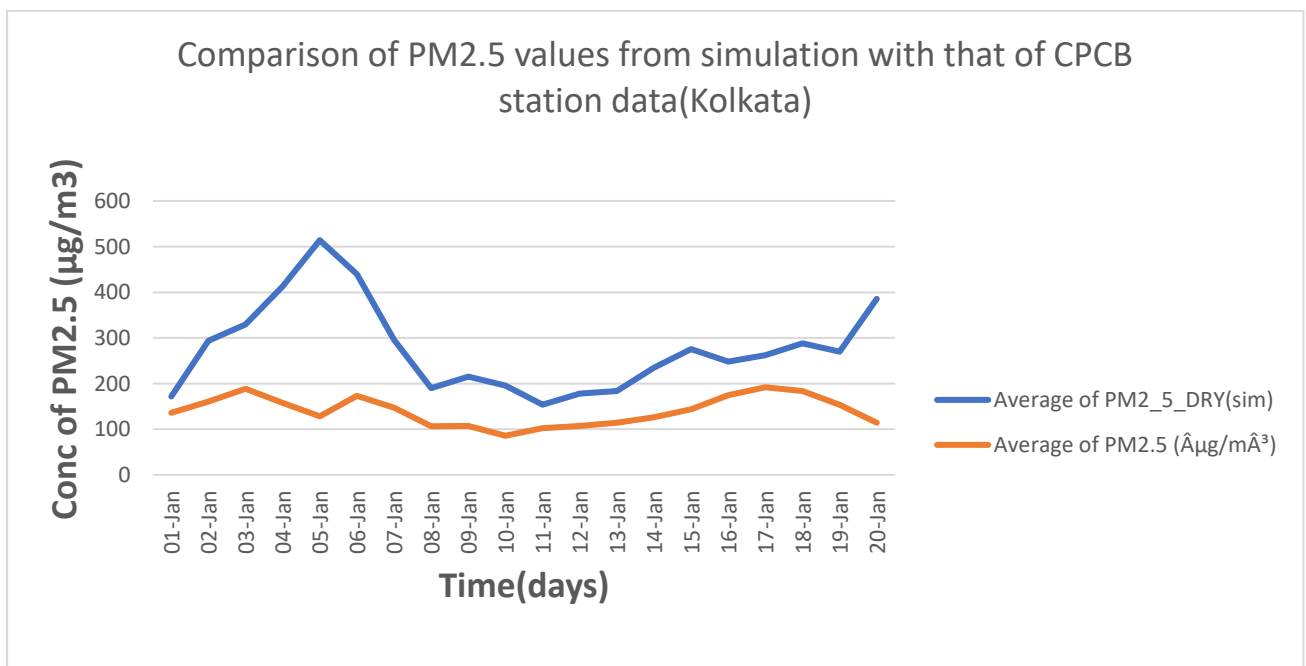


Comparison of PM<sub>10</sub> values from simulation with that of CPCB station data(TATA Stadium Joraphokhar)

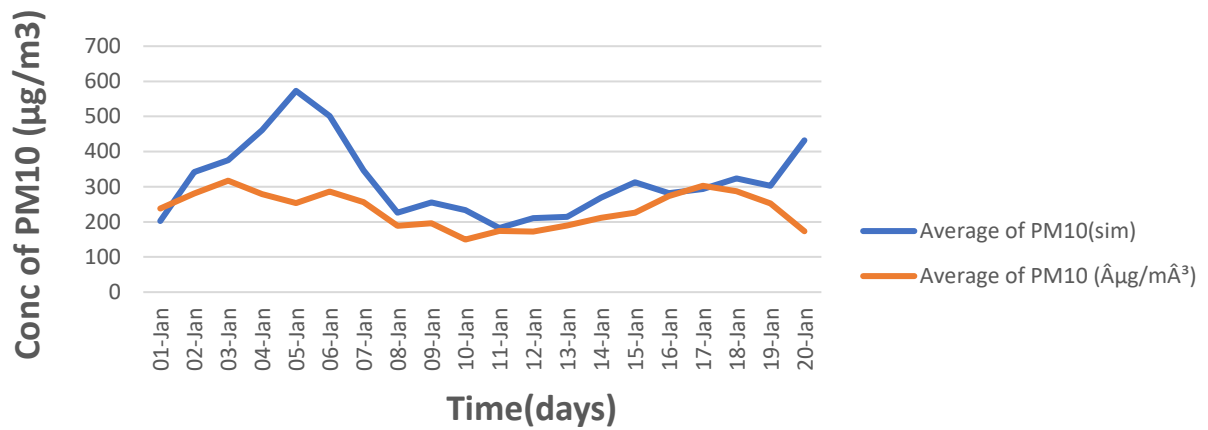




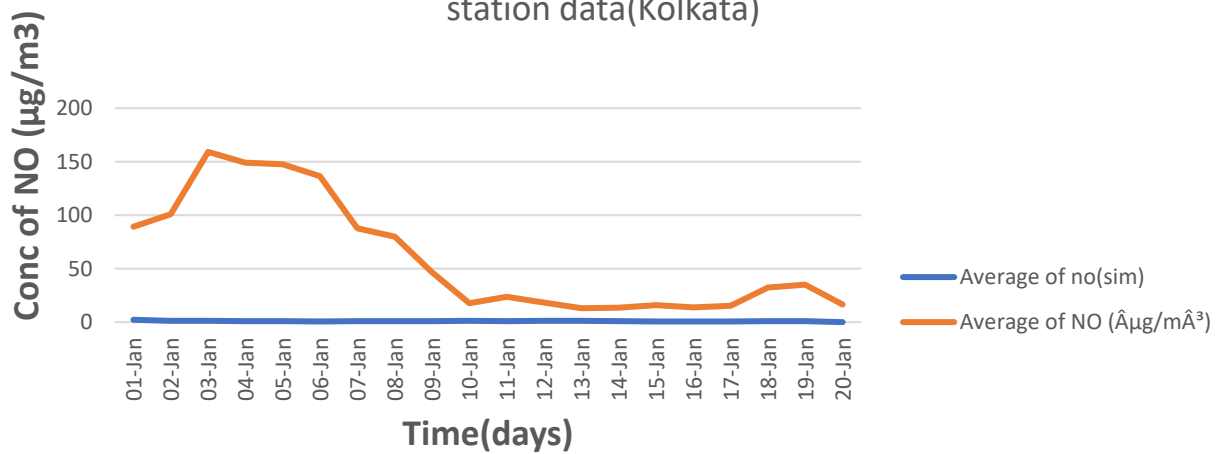
### C)Jadhavpur-Kolkata monitoring station

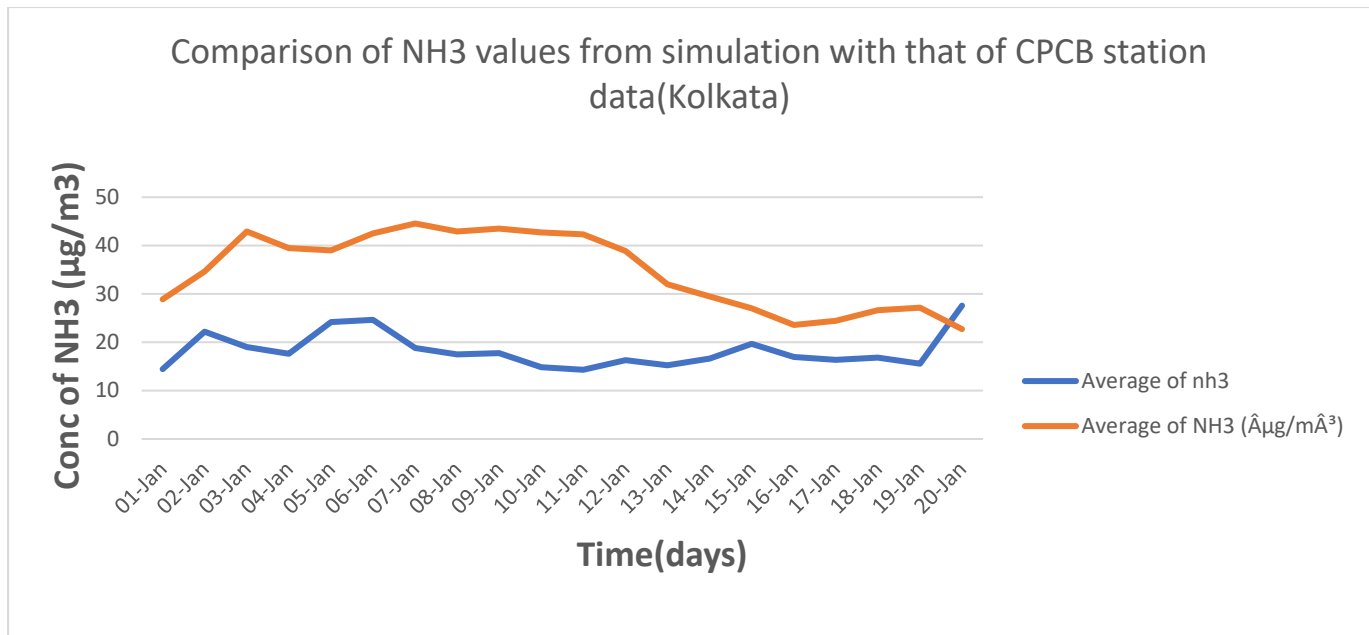


Comparison of PM10 values from simulation with that of CPCB station data(Kolkata)



Comparison of NO values from simulation with that of CPCB station data(Kolkata)





## 7. Discussion

### 7.1. Gas-Phase Pollutants Comparison

- **NH<sub>3</sub>, NO and NO<sub>2</sub>:** The model captured daily variations reasonably well, though underestimated peak concentrations.
- **O<sub>3</sub>:** Overprediction was observed during afternoon hours due to excessive photochemical activity.
- **SO<sub>2</sub> & CO:** Simulated values aligned well with observations, indicating accurate emissions representation.

### 7.2. PM<sub>10</sub> and PM<sub>2.5</sub> Comparison

- **PM<sub>10</sub> and PM<sub>2.5</sub>:** The model exhibited moderate agreement with CPCB data, with biases during high pollution episodes.
- Overestimation in regions with strong emission sources could suggest issues in emission inventory scaling.