Chapter 3

Inter-comparison of HTAP model simulation with satellite data and ground observations.

3.1 Introduction

In this chapter model simulated ozone and its precursors over the South Asian region is compared with available satellite data and ground observations. The ensemble-mean of fourteen HTAP models Phase 1 receptor base simulation (SR1) are used for the inter-comparison study.

Previous studies have shown that model simulation and observation differences can be due to both combination of model and observation errors. The uncertainty in the model input data (emissions, initial and boundary conditions, meteorology) some time leads to difference in model simulation and observation [Beckmann & Derognat, 2003]. The errors in satellite observations are due to errors in the cloud and aerosol characterization and surface albedo used for the retrievals [Blond et al., 2007].
Comparison of in-situ measurements of $O_3$ and CO profiles over Chennai, south India during the Indian summer monsoon of 2008 shows good agreement with WRF-Chem simulated $O_3$ and CO [Ojha et al., 2015]. GOME and SCIAMACHY satellite observation during the 1996 to 2006 period clearly detect high $NO_2$ column amount over the individual large thermal power plants over India [Ghude et al., 2009]. Over SA the WRF-Chem model simulation underestimates TES ozone and MOPITT CO except during August–January. WRF-Chem model simulated was able to generate the seasonal cycle of Surface $O_3$ and CO over SA, but $NO_x$ show some differences [Kumar et al., 2012].

Global simulation of $O_3$ and its precursors by MOZART model succesflly captured the observed values and seasonal cycle of ozone by ozonesondes, aircraft, and surface-monitoring stations [Horowitz et al., 2003]. Study by [Beig et al., 2007] over a semi urban site Pune in India shows a reasonable qualitative agreement with surface observation and MOZART-2 model results. Study done by [Wang et al., 1998] show that global three dimensional model generally capture the seasonal variation and the regional distribution of $O_3$, NO, PAN, $HNO_3$, CO, ethane, acetone and $H_2O_2$ observed by surface, ozonesonde, and aircraft observation. Global three-dimensional chemistry transport model study on bio-mass burning show that model results are comparable to ground based and aircraft CO observation at the region of bio-mass burning [Meredith Galanter & Carmichael, 2002]. The regional chemistry-transport model simulated CO over India shows similar feature observed by the MOPITT satellite data but the positions of the maximum concentrations of CO do not exactly match with the model simulation [Roy et al., 2008].

In this chapter, satellite retrieved Total Tropospheric Column Ozone (TTCO) is compared with the TTCO calculated from the model. For CO comparison, MOPITT satellite data is used. Total tropospheric column $NO_2$ data of SCIAMACHY satellite is used for the comparison of model simulated $NO_2$. Surface observation of four Indian station Observations over these stations were made with Air Quality Management System (AQMS) under the project Modeling Atmospheric Pollution and Networking (MAPAN).
3.2 Methodology

The main focus of this Chapter is to validating the ensemble mean of fourteen HTAP model over SA. The O₃ mixing ratios at different model levels are integrated from the surface to the tropopause to obtain the model TTCO. The formula in [Sheel et al., 2010] (equation 3.1) is used to calculate O₃ column

$$ TTCO = \int X(z) \cdot N_{air}(z) \cdot dz = \int X(z) \cdot \frac{A_{air}(z)}{M_{air}} \cdot dz $$  \hspace{1cm} (3.1)

Where \( N_{air}(z) \) is number density profile, \( M_{air} \) is mass density profile and molecular mass of air (in \( kgmol^{-1} \)). \( A_{air}(z) \) is the Avogadro’s number and \( X(z) \) is the O₃ mixing ratio.

There are two distinct way to determine the tropopause height 1. Height of the thermal tropopause 2. Height of the ozone tropopause. The WMO definition of tropopause is the lowest height at which the temperature lapse rate decreases to 2°K \( km^{-1} \) or less. Tropopause is also characterized by a sharp gradient in potential vorticity(PV). The PV value between 1.6 and 2 PV is defined as dynamical tropopause.

There are three criteria to determine the ozone tropopause height

1. Vertical gradient in ozone mixing ratio exceeds 60 ppbv km⁻¹.

2. Ozone mixing ratio greater than 80 ppbv. Given a typical O₃ ratio of 40-50 ppbv/pvu at the tropopause [Beekmann & Ancellet, 1994] this corresponds to a range of PV values between 1.6 and 2 pvu, consistent with definitions of the dynamical tropopause.

3. Ozone mixing ratio immediately above the tropopause exceeds 110 ppbv. This criterion rejects layers of stratospheric air in the troposphere where the maximum mixing ratio is less than 110 ppbv [Bethan et al., 1996].
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It is important to identify the proper tropopause height to avoid stratospheric air in the TTCO calculation, as the tropopause height changes with latitude and season. We calculate the total tropospheric column ozone using the criterion of rejecting the ozone mixing ratio greater than 110 ppbv. Thus for this calculation, we use an ozone-based tropopause and consequently O$_3$ concentration in the troposphere-stratosphere region exceeding 110 ppbv were ignored.

### 3.3 Comparison between model and satellite observation for O$_3$ CO and $NO_x$ over South Asia

The area averaged TTCO from satellite and model ensemble-mean for SA is shown in Figure 3.1.a. The seasonal cycle of TTCO generated by the models over SA is comparable with satellite observations, but the O$_3$ concentration is much greater in the models over SA, except in the months of April and May.

The spatial pattern of the difference between model simulated and satellite observed TTCO over SA for Pre-monsoon, Monsoon and Post-monsoon is shown in Fig. 3.2. The models show higher value of TTCO over SA in respect to Satellite except in pre-monsoon. During Pre-monsoon the model is showing lower value of TTCO over most part of India. Over most part of SA the difference between the model simulation and the satellite observation ranges from 0 to ±6 DU except over the Himalayan region. In all three seasons the models show much higher O$_3$ over the Himalayan region. This may explain the higher value of area averaged O$_3$ column over SA in the models than satellite observation in Fig 3.1.

Moppit surface CO data is averaged over SA to compare with model simulated CO which is shown in Figure 3.1.b. Model and Satellite is showing similar seasonal cycle, but with a shift of one month. Model is showing minimum value of CO in month of June but satellite observation shows minimum value in July. From the seasonal cycle we can say that satellite is showing much more higher value of CO in winter and Pre-monsoon in respect to monsoon and Post-monsoon.
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Spatial pattern of difference between model simulated and satellite observed surface CO over SA 3.3 shows almost similar pattern. In pre-monsoon satellite is showing high value over Indo-gangetic plane with respect to the model simulation. Indo-gangetic plane is most populated and highly industrial region of SA. Studies like [Clerbaux et al., 2008] show that CO signal arising from cities might some extent be enhanced by the specific dynamic and thermal conditions occurring over urban areas, generally known as heat island effect. Such effects may be a reason for the difference between model results and satellite data.

Area averaged Total tropospheric column $NO_2$ data of SCIAMACHY satellite over SA is compared with model simulated $NO_2$ (shown in Figure 3.1.c). Satellite is showing quite high value compare to model simulation in the months of August to December. The spatial pattern of $NO_2$ (Figure 3.3) does not match
between model and satellite although the values are in range. Along the Indo-
igangetic plane model having high value of $NO_2$ but satellite is not showing such
signature there.

### 3.4 Comparison between model simulation and surface observations

The four stations considered show minimum surface $O_3$ values in the monsoon
period and maximum values in the pre-monsoon. The seasonal variation of surface
$O_3$ over the four stations is shown in Figure 3.4. Monthly averages of observations
taken each hour is compared with ensemble mean surface $O_3$ from the models
over the corresponding station location. The model simulations reproduce the
seasonal cycle of surface $O_3$ concentration over the locations, but are substantially
higher. The ground-level ozone mixing ratios from the models have been examined

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**Figure 3.2:** Difference between model simulation and satellite ob-
servation of total tropospheric $O_3$
column for (a) Pre-monsoon (b) Mono-
soon (c) Post-monsoon.
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Collectively as an ensemble and evaluated against a large set of observations from both Europe and East Asia [Fiore *et al.*, 2009]. This commonly used multi-model approach can be outperformed by subsets of models optimally selected in terms of bias, error, and correlation, but it does not strictly depend on the skill of individual models, although it may require the inclusion of low ranking skill score members [Solazzo *et al.*, 2012].

The difference between the models and surface observations may be due to the fact that the global models are not able to capture fine-scale emission patterns at the coarse resolutions used here. A further reason may be that the relatively low sampling height (3m) of observations does not match the elevation of the middle...
of each model's grid box. An earlier analysis by [Van Dingenen et al., 2009], comparing 30 meter and 10 meter concentrations, showed that in India this may lead to overestimation of the order of 20–30 ppb. Such bias may be even higher when comparing with 3m. Another reason for this difference may be that over India $NO_x$, one of the most important precursors of $O_3$ is strongly affected by local emissions. Biomass and fossil fuel burning is the main source of $NO_x$ over this region. Due to the increasing population and higher economic growth rates, emission of these gases are increasing over SA [Akimoto et al., 2003, Sheel et al., 2010]. Surface observations of $NO_x$ over these four stations are much higher (5-17 ppbv) than in the model simulations (0.1-2 ppbv). This suggests that destruction of $O_3$ by direct reaction with emitted NO is much more important than seen in the models, accounting for the overestimation of surface $O_3$ in the models.
3.5 Comparison between model and satellite observation at station locations

The seasonal variation of ensemble mean TTCO over station locations (generated by interpolating the gridded data to the exact station locations) is compared with satellite data in Figure 3.5. The model results are consistent with the satellite observations but show systematically higher O$_3$ values (35–45 DU) in monsoon months (June–September) relative to the satellite observations (27–40 DU), whereas in the dry months the bias is much smaller (1–5 DU). The difference in O$_3$ column between satellite observations and model simulations may be due to the fact that in monsoon months, the thick clouds in the field of view obscure the infrared emission from the lower troposphere, which greatly reduces TES sensitivity [Nassar et al., 2008]. There is also missing satellite data over some parts of Asia in monsoon months. The model columns over the four stations are more consistent with the satellite observations because over most part of SA the
difference between the model simulation and the satellite observation ranges from 0 to 6 DU.

\[\text{Fig. 3.6: Seasonal variation of the total tropospheric CO column from model simulation and satellite observation over Hyderabad, Pune, Jabalpur and Udaipur.}\]

Seasonal variation of Total Tropospheric \(\text{NO}_2\) satellite data is compared with model date over the four Indian station locations (Figure 3.6). In the post-monsoon months the satellite is showing much higher value in respect to model simulation. The variation seasonal cycle of satellite is quite large (ranges from 2 to \(5.5 \times 10^{15}\) molecule/cm\(^2\) in respect to model which ranges from 2 to \(3.5 \times 10^{15}\) molecule/cm\(^2\). Both model and satellite is showing higher values of \(\text{NO}_2\) in post-monsoon season.

Over this four station the surface CO of MOPITT satellite is compared with the model simulated CO (Figure 3.6). The seasonal cycle of CO of Model and Satellite is consistent to each other with. Similar to area averaged seasonal cycle over SA satellite is showing higher value in winter and pre-monsoon and lower in post-monsoon with respect to model simulation. The difference between model and satellite is minimum in monsoon.
3.6 Summary and discussions

Comparison between model simulations, satellite observations and surface observations show some discrepancy in O$_3$ and its precursors concentration and seasonal variation. Possible reasons for the discrepancies are error in satellite measurement, coarse model resolution which alters chemical timescales and prevents like-for-like comparison with observations, and high temperatures and humidity over SA which can shorten chemical timescales. The uncertainty in the model input data like emission inventories, initial and boundary conditions and meteorology some time leads to difference in model simulation and observation. The errors in satellite observations are due to errors in the cloud and aerosol characterization and surface albedo used for the retrievals may also leads to the discrepancy. Hence biases in O$_3$ formation are larger in SA than elsewhere. Satellite observations of total tropospheric O$_3$ column over SA show much better agreement, but are generally biased low by 5–10 DU, except in May month. Surface observations over four Indian stations show much lower values of O$_3$ compared to the model simulations but the TTCO obtained from satellite is relatively consistent with that from the model simulations. Seasonal cycle and magnitude of model simulation and satellite is consistent. The spatial pattern of model simulated Total tropospheric NO$_x$ and satellite observation does not matches well but there magnitude is almost same. The discrepancy in O$_3$ and its precursor may lead to uncertainty in the attribution of foreign contributions to pollution over this region, but there is no reason to believe that the foreign fraction is the cause of discrepancies.