EMS Annual Meeting Abstracts
Vol. 13, EMS2016-586, 2016
16th EMS / 11th ECAC

Validation of WRF/Chem Model and Sensitivity of Chemical Mechanisms to Ozone Simulation over Megacity Delhi

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Regional Chemical transport models (CTM) are used extensively for modeling of Ozone concentration. WRF/Chem is one such CTM that includes various chemical mechanisms and is used for simulation of Ozone and other pollutant concentration at desired time step. This study focuses on the robustness of WRF/Chem simulated Ozone concentrations over a sub-tropical urban airshed of megacity Delhi. Detailed analysis has been presented for the veracity of two different chemical mechanisms namely; Carbon Bond Mechanism (CBMZ) and Regional Atmospheric Chemical Model (RACM). It was observed that simulated Ozone concentrations are better predicted with CBMZ mechanism and is highly sensitive to the rate constants. The value of statistical parameter RMSE (Root Mean Square Error) for modeled Ozone concentration with CBMZ mechanism was 32.97 μg m-3 and for RACM was 40.13 μg m-3. Similarly, value of IOA (Index of Agreement) was also better for CBMZ (0.82) in comparison to RACM (0.55). The Ozone concentrations are analyzed for precursors such as Oxides of Nitrogen (NO_x) and Carbon-monoxide (CO) as well as temperature considering their strong dependence on Ozone formation. A consistent positive correlation between Ozone concentration and temperature is noted whereas; NO_x and CO show inverse relationship with Ozone. Further, Ozone concentration range vis-à-vis model performance is scrutinized. A poor model for low Ozone concentration levels is observed and a highly satisfactory for moderate Ozone concentration levels while satisfactory for higher Ozone levels. Despite of the limitations observed during model evaluation of Ozone predictions for low Ozone levels, it is concluded that WRF/Chem could effectively be applied for understanding its trends, tropospheric chemistry and air quality assessment for regulatory purposes at moderate Ozone concentration levels. Further, it is recommended that model implementation shall be made for policy decisions cautiously with due consideration to the magnitudes of Ozone levels present in the study domain and the performance measures in the specific concentration range.