Modeling diurnal variation of surface $PM_{2.5}$ concentration over East China with WRF-Chem: Impacts from boundary layer mixing and anthropogenic emission

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Diurnal variation of surface $PM_{2.5}$concentration (diurnal $PM_{2.5}$) could dramatically affect aerosol radiative and healthy impact, and can also well reflect the physical and chemical mechanisms of air pollution formation and evolution. So far, diurnal $PM_{2.5}$and its modeling capability over East China has not been investigated, and therefore, is examined in this study. Based on the observations, the normalized diurnal amplitude of surface$PM_{2.5}$concentrations averaged over East China is the weakest (˜1.2) in winter, and reaches ˜1.5 in other seasons. The diurnal $PM_{2.5}$shows the peak concentration during the night in spring and fall and during the daytime in summer. The simulated diurnal $PM_{2.5}$with WRF-Chem and its contributions from multiple physical and chemical processes are examined in the four seasons. The simulated diurnal $PM_{2.5}$with WRF-Chem is primarily controlled by planetary boundary layer (PBL) mixing and emission variations, andis significantly overestimated against the observation during the night. This modeling bias is likely primarily due to the inefficient PBL mixing of primary $PM_{2.5}$during the night. The simulated diurnal $PM_{2.5}$is sensitive to the PBL schemes and vertical layer configurations with WRF-Chem. Besides the PBL height, the PBL mixing coefficient is also found as the critical factor determining the PBL mixing of pollutants in WRF-Chem. With reasonable PBL height, the increase of lower limit of PBL mixing coefficient during the night can significantly reduce the modeling biases in diurnal $PM_{2.5}$and also the mean concentrations, particularly at the major cities of East China. It can also reduce the modeling sensitivity to the PBL vertical layer configurations. The diurnal variation and injection height of anthropogenic emissions also play roles on simulating diurnal $PM_{2.5}$, but the impact is relatively smaller than that from the PBL mixing. This study underscores that more efforts are needed to improve the boundary mixing process of pollutants in models with observations of PBL structure and mixing fluxes in addition to PBL height, in order to simulate reasonably the diurnal $PM_{2.5}$over East China. The diurnal variation and injection height of anthropogenic emissions are also necessary to be included to simulate the diurnal $PM_{2.5}$ over East China.

Keywords: WRF-Chem, PBL mixing, diurnal cycle