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PC13) Dispersion and Photochemical Oxidation of Reduced Sulfur Compounds in and around a Large Industrial Complex in Korea

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1. Introduction

In this study, the photochemical oxidation of reduced sulfur compounds(RSCs) was investigated using the RSC concentration data set measured from a number of urban locations surrounding a large-scale industrial complex(i.e., Ban-Wall industrial complex(BWIC)) during several field campaigns held in 2004-2005(Choi et al., 2006; Kim et al., 2006). Based on these field measurement data and the abbreviated oxidation mechanisms of RSCs, model calculations for photochemical oxidations of RSCs were conducted in this study. In addition, the dispersion of RSCs emitted from industrial sources was assessed using the CALPUFF modeling system. We intended to assess the contribution of RSCs emitted from industrial regions to SO_2 concentration levels in the surrounding regions. The details of our initial effort to characterize the spatial and temporal distributions of RSCs in the same study area have been reported elsewhere(Pal et al., submitted).

2. Model descriptions

To assess how SO_2 distribution is affected by RSC emissions from the BWIC, the chemical transformation mechanism of the five RSCs was added to the CALPUFF dispersion model system (with RIVAD/ARM3 chemical scheme: Morris et al., 1988). Moreover, the PSU/NCAR no-hydrostatic meteorological model(i.e., MM5) was used to simulate a meteorological field together with four dimensional data assimilation(FDDA) as the initial meteorological field to CALMET. The FDDA technique was applied to the CALMET based on specific meteorological variables(e.g., air temperature, wind direction, and speed) from 7 Automatic Weather System(AWS) in the entire study area. The computational domain in MM5 consisted of 23 sigma vertical levels and 55×55 grid points in a horizontal grid size resolution of 27 km on the following domain: 24.2-49.5°N, 114.8-140.6 °E with the center at 36.8°N, 127.7°E. The whole study area was nested as four domains(i.e., 27×27, 9×9, 3×3, and 1×1km) using the two-way nesting method. The initial field and boundary conditions were extracted from Regional Data Assimilation and Prediction System(RDAPS) data. The RDAPS was produced from the MM5 model simulation with horizontal resolutions of 30km(191×171 grids) and 33 levels of vertical terrain-influenced coordinates with the center at 38°N, 126°E.

For our numerical modeling, the abbreviated oxidation mechanisms of RSCs and their emissions were added to the section of chemical transformation. The 34 dominant chemical reactions of RSCs were used in this study to predict the SO_2 concentrations arising from the RSC oxidation mechanisms, as described previously in Shon and Kim(2006). The contribution of the RSC oxidation to SO_2 budget was estimated by simultaneously considering the emission of RSCs and SO_2.

3. The role of RSC on the formation of SO_2 in and outside of the BWIC

Fig. 1 shows surface distributions of SO_2 with mostly northwesterly and easterly surface winds of approximately 1 to 10m s^{-1}. The SO_2 concentrations at the surface level hence depend on the wind speed and direction of the inflow of winds. A land-sea breeze circulation was dominant during summer and fall(i.e., a strong sea breeze in the afternoon and a weak land breeze in the early morning), whereas synoptic-scale winds were prominent during winter(i.e., a very weak land-sea breeze circulation). During summer(Fig. 1a), high SO_2 concentrations converged into the source regions(i.e., the BWIC) in the early morning(i.e., at 0900 Local Standard Time(LST)) it was however found to move into the southeastern areas from the BWIC in the afternoon (i.e., at 1500 LST). In particular, SO_2 concentration levels at 0900 LST reached significantly high levels of approximately 100 ppbv in the central BWIC along with the convergence of wind at low wind speed(e.g., 2m s^{-1}). During winter(Fig. 1b), a relatively low SO_2 concentration(maximum of 20ppbv) was observed persistently in downstream regions(the southeastern area from the BWIC) at both 0900 and 1500 LST due to the dilution effect predominated by the strong synoptic-scale winds(e.g., northwesterly) at approximately 10m s^{-1}. During fall, SO_2 concentration levels of 30ppbv were dominant in downwind regions(the northwestern area from the BWIC) with the inflow of southerly and/or southeasterly winds(Fig. 1c).

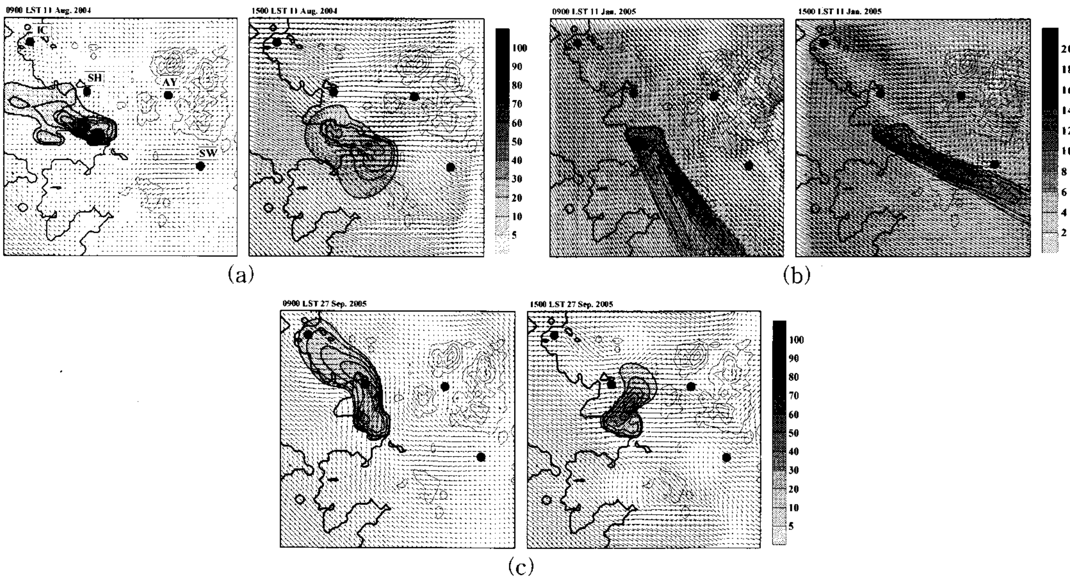

Fig. 1. Horizontal distributions of the simulated wind vectors(m s^{-1}) and SO_2 concentrations(ppbv) at 0900 and 1500 LST during (a) summer, (b) winter, and (c) fall study period. The names of city shown in the figure are abbreviated as follows: IC=In Cheon; SH=Si Heung; AY=An Yang; and SW=Su Won.

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