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1,3-butadiene in urban and industrial areas and its role in photochemical processes

Beata Czader and Bernhard Rappenglück
University of Houston, Department of Earth and Atmospheric Sciences, Houston, United States (brappenglueck@uh.edu)

1,3-butadiene is an important pollutant in terms of public health and important driver for photochemical processes influencing ozone formation in the area of Houston. Ambient levels of 1,3-butadiene were simulated with the Community Multiscale Air Quality model (CMAQ) including the SAPRC99-extended mechanism and the results were compared to spatially and temporally resolved observations of 1,3-butadiene for an episodic period during Summer 2006. Relative contributions of different type of emissions and chemical reactions to 1,3-butadiene concentrations were examined, the highest contribution was found to be from industrial emission sources. 1,3-butadiene mixing ratios in the urban area were found to be lower than in the industrial area. Although emissions of 1,3-butadiene peak during daytime its mixing ratios are lower during daytimes as compared to nighttime. 1,3-butadiene is removed from the surface through vertical upward transport ($\sim$90%) and chemical reactions ($\sim$10%). During daytime 1,3-butadiene reacts mainly with the OH radical (90%), during nighttime this reaction pathway is still significant in the industrial area (57% of all reaction pathways). Reaction with NO_3 during nighttime contributes 33% in industrial and 56% in urban areas, where high NO_x emissions occur. Reaction with ozone contributes 10% and 13% in industrial and urban areas, respectively. Analysis of measured data revealed that episodically very high emissions spikes of 1,3-butadiene occur. CMAQ often underpredicts 1,3-butadiene mixing ratios when sites are exposed to sporadic releases from industrial facilities. These releases are not accounted for in the emission inventory. It also appears that emissions of 1,3-butadiene from point sources have much more variability than those listed in the emission inventory.