EMS Annual Meeting Abstracts Vol. 10, EMS2013-229, 2013 13th EMS / 11th ECAM © Author(s) 2013



Large-Eddy Simulation of Pollutant Dispersion from a Ground-Level Area Source over Urban Street Canyons with Irreversible Chemical Reactions

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Most air pollutants are chemically reactive in which the complex reactions among different species cannot be neglected. Pollutant distribution is mainly governed by flows and turbulent mixing. In the canopy layer over urban areas (UCL), in which the turbulence intensities are affected by both the atmospheric conditions and the rough urban surfaces at the bottom, makes the situation more complicated.

In this study, the dispersion of chemically reactive pollutants is calculated by large-eddy simulation (LES) in a neutrally stratified UCL. The computational domain, representing a hypothetical urban area, consists of 36 repeated street canyons placed in cross flows. As a pilot attempt, street canyons of building-height-to-street-width (aspect) ratio of unity are used. Nitric oxide (NO), one of the major vehicular pollutants, is emitted from the ground surface of the first street canyon that is transported downstream in the prevailing wind direction in the form of pollutant plume. The domain is doped with ozone (O_3) which oxidizes NO to produce nitrogen dioxide (NO₂). This chemical reaction is irreversible in the absence of ultraviolet and the reaction rate is assigned to be a constant.

A range of turbulence time scales and reaction time scales are utilized to examine the mechanism of turbulent mixing and chemical reactions in the UCL. NO generally decreases in the streamwise direction because of both turbulent dilution and titration with background O_3 . Using the LES results, we attempt to demystify the key pollutant removal mechanism over urban areas in different configurations of building morphology and pollutant sources.