Atmospheric Chemistry Reactions in a Turbulent Flow: Application to an Urban Environment

The understanding of air chemistry in atmospheric flows in planetary boundary layer is vital in learning the dispersion and reaction of pollutants in the air. In the absence of turbulence, originally segregated chemically reactive trace gases advect without interacting. When turbulence is taking place, a cascade of motions appears and leads to small-scale mixing of the tracers and therefore chemical reactions. For the reactions with the turbulent timescale longer than the chemical timescale, the chemistry is said to be fast. The tracers react in a lower rate as if they are well-mixed. Chemical-turbulence interaction is considered to be a sub-grid process, and is unresolved in large-scale models. Turbulent mixing of chemicals in the air is then parameterized. However, these parameterization schemes are too simplified, resulting in miscalculation of the resultant tracer production. A better representation of the sub-grid chemical-turbulence interaction is necessary for sophisticated air quality monitoring and prediction.

In order to study the problem, tracer advection simulations in turbulent wind field have been conducted in both two- and three-dimensions, with the simulation domain mimicking a grid in a large-scale chemical transport model. A simple chemistry scheme was implemented to calculate the effective chemical reaction rate. Simulations in set of three variables, namely the Reynolds number, the chemical reaction rate coefficient and the initial separation between the reactant tracers were performed. The results were then compared with an unresolved model, in which the tracers were assumed to be well-mixed inside the simulation domain. Both the tracer segregation and production in the resolved model significantly differed from the values in the unresolved model, when the Damköhler number, i.e. the ratio between the turbulent and chemical timescales, is large.

The investigation is then continued by studying turbulent reacting flows in the planetary boundary layer (PBL) through direct numerical simulations (DNS) and large eddy simulations (LES). The interaction of turbulent motion in PBL and tracer chemistry with tropospheric ozone production has been studied in simple chemistry scheme and emission configurations to depict the real-life situations in urban areas. Here some preliminary results of the DNS and LES simulations are presented. At last, high-resolution coupled LES simulations will be conducted in the setting of the urban area of Hong Kong. The urban topography and inhomogeneous emission in the city will be implemented on existing models. The results will then be compared with observational data and other related studies conducted in other scales.