Atmospheric Environment 75 (2013) 153–162

Contents lists available at SciVerse ScienceDirect

Atmospheric Environment

journal homepage: www.elsevier.com/locate/atmosenv

Large-eddy simulation coupled to mesoscale meteorological model for gas dispersion in an urban district

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HIGHLIGHTS

- A microscale LES model was coupled to a mesoscale LES model.
- The LES without combing the mesoscale model overestimated the gas concentration.
- The present LES predicted the gas concentration within an actual urban district.

ARTICLE INFO

Article history:
Received 26 December 2012
Received in revised form
7 March 2013
Accepted 8 April 2013

Keywords:
Atmospheric dispersion
Large-eddy simulation
Meteorological influence
Urban district
Field measurement

ABSTRACT

A microscale large-eddy simulation (LES) model coupled to a mesoscale LES model is implemented to estimate a ground concentration considering the meteorological influence in an actual urban district. The microscale LES model is based on a finite volume method with an unstructured grid system to resolve the flow structure in a complex geometry. The Advanced Regional Prediction System (ARPS) is used for mesoscale meteorological simulation. To evaluate the performance of the LES model, 1-h averaged concentrations are compared with those obtained by field measurements, which were conducted for tracer gas dispersion from a point source on the roof of a tall building in Tokyo. The concentrations obtained by the LES model without combing the mesoscale LES model are in quite good agreement with the wind-tunnel experimental data, but overestimates the 1 h averaged ground concentration in the field measurements. On the other hand, the ground concentrations using the microscale LES model coupled to the mesoscale LES are widely distributed owing to large-scale turbulent motions generated by the mesoscale LES, and the concentrations are nearly equal to the concentrations from the field measurements.

1. Introduction

With the increasing availability of powerful supercomputers, numerical simulations have become an attractive tool for simulating transport and dispersion of airborne materials in an urban district. Microscale computational fluid dynamics (CFD) methods such as Reynolds-averaged Navier–Stokes (RANS) simulation and large-eddy simulation (LES) are often used to predict velocity and concentration fields in an urban district. Concentrations averaged over 3–10 min can usually be estimated by wind-tunnel experiments (e.g., Nakayama and Nagai, 2009; Michioka et al., 2011a), but estimates of tens of minutes are not possible because meteorological influences such as a wind direction and large-scale buoyancy-driven motions (Castillo et al., 2011) cannot be generated by these normal CFD methods. Longer estimates are important, however, because 1 h averaged concentrations are generally used for environmental impact assessments in Japan, for example. To incorporate such meteorological influences into CFD, large-scale turbulent motions need to be generated in some way.

When simulating airflow and gas dispersion considering meteorological influence, one of the most suitable tools is a microscale (less than a few kilometers in horizontal extent) CFD coupled with a mesoscale meteorological model. Kondo et al. (2006) conducted RANS simulation combined with various boundary conditions for diffusion of NO_x around a heavily polluted roadside in Tokyo, Japan (the Ikegami-Shinmachi crossroads). They tested three types of lateral boundary conditions: (1) a mesoscale meteorological model, (2) local one-point observations, and (3) wind conditions were given with the observation, and conditions for the turbulent kinetic energy and the dissipation rate were given with the inferred values from a mesoscale meteorological model. They showed that the concentration of NO_x with the first boundary condition using the

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http://dx.doi.org/10.1016/j.atmosenv.2013.04.017

mesoscale meteorological model appears better than the other boundary conditions. However, RANS simulation using a microscale CFD model has the following weaknesses. The boundary conditions of the turbulent kinetic energy and dissipation rate must be given using models, because these parameters are not calculated in the mesoscale meteorological model. In addition, RANS simulation cannot predict gas dispersion accurately because it is affected not only by the mean flow, but also by the turbulence and scalar fluctuations. The turbulent Schmidt number, which strongly affects the turbulent scalar flux, is the tunable parameter appearing in the turbulent scalar flux model (Tominaga and Stathopoulos, 2007; Michioka and Sato, 2009). Hence, RANS simulation can predict the concentration in only the case that an optimal empirical value of the turbulent Schmidt number is chosen.

On the other hand, LES does not significantly depend on the subgrid-scale turbulent Schmidt number, which is also a tunable parameter, and can accurately reproduce flow and gas dispersion in an urban district, provided the mesh resolution is sufficient. In addition, LES can accurately reproduce the coherent structure of low-momentum fluid above urban canyons, which strongly affect gas dispersion (Michioka et al., 2011b; Michioka and Sato, 2012).

Nozu and Tamura (2012) conducted LES for gas dispersion emitted from a point source on the ground in a large city, namely Tokyo, and indicated that the LES can reproduce the time-averaged concentration obtained by wind-tunnel experiments. Xie and Castoro (2009) used LES to examine flow and dispersion within an urban area in Central London (at a DAPPLE Project site), and demonstrated that mean and root mean square (rms) concentrations predicted by LES with full-scale resolution of around 1 m are in reasonable agreement with wind-tunnel experimental data. In addition, Xie (2011) used meteorological wind conditions measured at the DAPPLE Project site as boundary conditions at 30 s intervals to drive numerical simulations of flows and dispersion, in which the turbulent fluctuations between the time intervals were reproduced by using an inflow generator (Xie and Castoro, 2008). The mean concentrations predicted by LES were in better agreement with the field measurements than when steady wind conditions were used. Liu et al. (2012) implemented LES to study the wind field and pollutant dispersion in an urban district in Beijing. The lateral and top boundary conditions were provided by the mesoscale meteorological model (Weather Research and Forecasting, WRF). The wind, temperature and carbon monoxide concentration predicted by the LES showed relatively good agreement with observation. However, they stated that further improvements were needed. LES requires instantaneous turbulent fluctuations under lateral boundary conditions, but boundary values were updated every 15 min because the mesoscale meteorological model provided only large-scale motions.

Most mesoscale meteorological models are based on RANS formulations, while the microscale LES model requires instantaneous values at the boundaries. To couple the microscale LES model with a mesoscale meteorological model, instantaneous turbulent flow at the lateral boundaries for the microscale LES model must be generated (Mochida et al., 2011; Yamada and Koike, 2011). On the other hand, there are methods using a mesoscale meteorological model based on the LES formulation. Chow et al. (2006) and Michioka and Chow (2008) applied the Advanced Regional Prediction System (ARPS) based on LES for mesoscale meteorological simulation. The differences between LES and RANS simulation become small when similar space and time resolutions are used; often the only difference in implementation is the formulation of the turbulence model. The advantage of the mesoscale LES model, however, is that the unsteady turbulent motions can be generated under the condition that the computational mixing is sufficiently small (Michioka and Chow, 2008).

The present study implements a microscale LES model coupled to a mesoscale LES model to estimate ground concentrations considering the meteorological influence in an actual urban district. A microscale LES model is based on a finite volume method with an unstructured grid system for resolving the flow structure in a complex geometry. The mesoscale meteorological model (ARPS), developed at the Center for Analysis and Prediction of Storms at the University of Oklahoma (Xue et al., 2000, 2001) was also used for mesoscale meteorological simulation. To evaluate the performance of the LES model, it was applied to simulate the dispersion of tracer gas released from the roof of a building at the Komae Research Laboratory, Central Research Institute of Electric Power Industry (CRIEPI), Japan, where field experiments were conducted on 3 February 2005.

2. Mesoscale meteorological model

The mesoscale meteorological model is an ARPS − a non-hydrostatic, compressible LES code written for mesoscale and small-scale atmospheric flows (Xue et al., 2000, 2001, 2003). ARPS solves equations for each velocity component, the perturbation pressure, potential temperature, and moisture. Density is diagnosed from an equation of state. Fourth-order spatial differencing is used for advection terms in the momentum, potential temperature, and pressure equations. Temporal discretization is performed by using a mode-splitting technique to accommodate high-frequency acoustic waves. Large time steps use the leapfrog method. First-order forward−backward explicit time stepping is used for small times steps, except for terms responsible for vertical acoustic propagation. The 1.5-order turbulent kinetic energy closure (TKE-1.5) was used for the subgrid-scale turbulence model for all prognostic variables on all domains.

ARPS is used for simulations of three tracer gas releases at Komae-shi, Tokyo, Japan, where a field campaign was conducted in 19 November 1989 (Sato et al., 2008). The concentration of the tracer gas is not solved in the mesoscale LES model because the background concentration of the tracer gas used in field experiments is nearly zero. The simulation begins at 21:00 JST (Japan standard time; UTC = JST − 9) of the day prior to the passive scalar release. The predominant wind direction was from the north.

Table 1 gives details of ARPS simulation domains. Six one-way nested grids were used to simulate flow and scalar dispersion around CRIEPI at horizontal resolutions of 24.3 km, 8.1 km, 2.7 km, 900 m, 300 m and 100 m (see Fig. 1). Topography for the 24.3 km–900 m grids was obtained using U. S. Geological Survey (USGS) 30-arc second topography datasets. The 300 m (and finer) resolution terrain data were extracted from a Japanese Geographical Survey Institute 50 m dataset. To obtain realistic initial and boundary conditions, data from the Japanese-25 year Reanalysis (JRA-25) dataset were used to force ARPS simulations on the coarsest-resolution (45 km) grid. JRA-25 analyses are given at 6 h intervals with 1.125° (approximately 135 km) horizontal spacing and 40 vertical levels (Onogi et al., 2007). Update intervals on subsequent

Table 1
Nested grid configurations with dimensions.

Region	Grid size	Domain (km)	Δx, Δy	$\Delta z_{\min}$	Update interval ΔT_b
1	83 × 83 × 53	1944 × 1944 × 25	24.3 km	50 m	6 h
2	83 × 83 × 53	648 × 648 × 25	8.1 km	50 m	10 min
3	83 × 83 × 53	216 × 216 × 25	2.7 km	50 m	10 min
4	83 × 83 × 53	72 × 72 × 20	900 m	30 m	10 min
5	83 × 83 × 53	24 × 24 × 17.5	300 m	20 m	5 min
6	83 × 83 × 53	8 × 8 × 16	100 m	10 m	10 s.