Yale-NUIST Center on Atmospheric Environment

Testing of a Large Eddy Simulation model on the NUIST super-computer

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Outline

- Introduction
- Scientific questions
- Methods
- LES case study
- Summary
- On-going work

Introduction

- The smoggy atmospheric boundary layer (ABL) as a new type of boundary layer plays an important role in the occurrence of heavy haze pollution events.
- To date, the structures of the ABL under smoggy conditions are not well understood (*Lee et al., 2015*).
- Large amount of aerosols with varying size are trapped or accumulated within the atmospheric boundary layer (from surface to up to 3 km) (*e.g., IPCC, 2007; Ramanathan et al., 2001*).

Introduction (cont.)

- Atmospheric aerosols affect the Earth-atmosphere radiation budget directly by scattering and absorbing the incoming solar radiation, and indirectly by modifying the cloud radiative properties through altering the cloud microphysical properties (*Kedia et al., 2010*).
- In general, atmospheric aerosols causes significant atmospheric radiative heating in solar wavelengths (SW) and cooling in long wavelengths (LW) (*Carlson and Benjamin, 1979; Quijano et al., 2000; Won et al., 2004*).
- Aerosol radiation effect may have different heating/ cooling rates at different layers within the ABL, and eventually modifies the atmospheric boundary layer structures. However, the impact of aerosol radiation effect on the ABL is not well quantified.

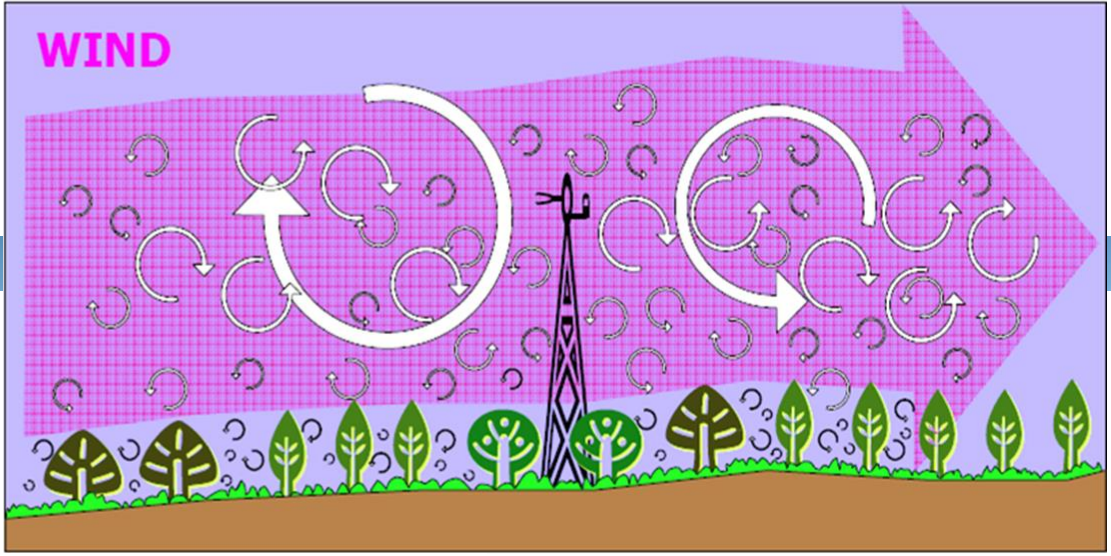
Introduction (cont.)

- Large Eddy Simulation (LES) model is a powerful tool to study the atmospheric boundary layer (*Deardorff 1972; Moeng 1984*).
- Current LES model does not include the aerosol radiative effect, which greatly limits the application of LES in the atmospheric boundary layer.
- The impact of aerosol radiation effect on the smoggy boundary layer will be investigated through the offline and online coupling LES/Aero system.

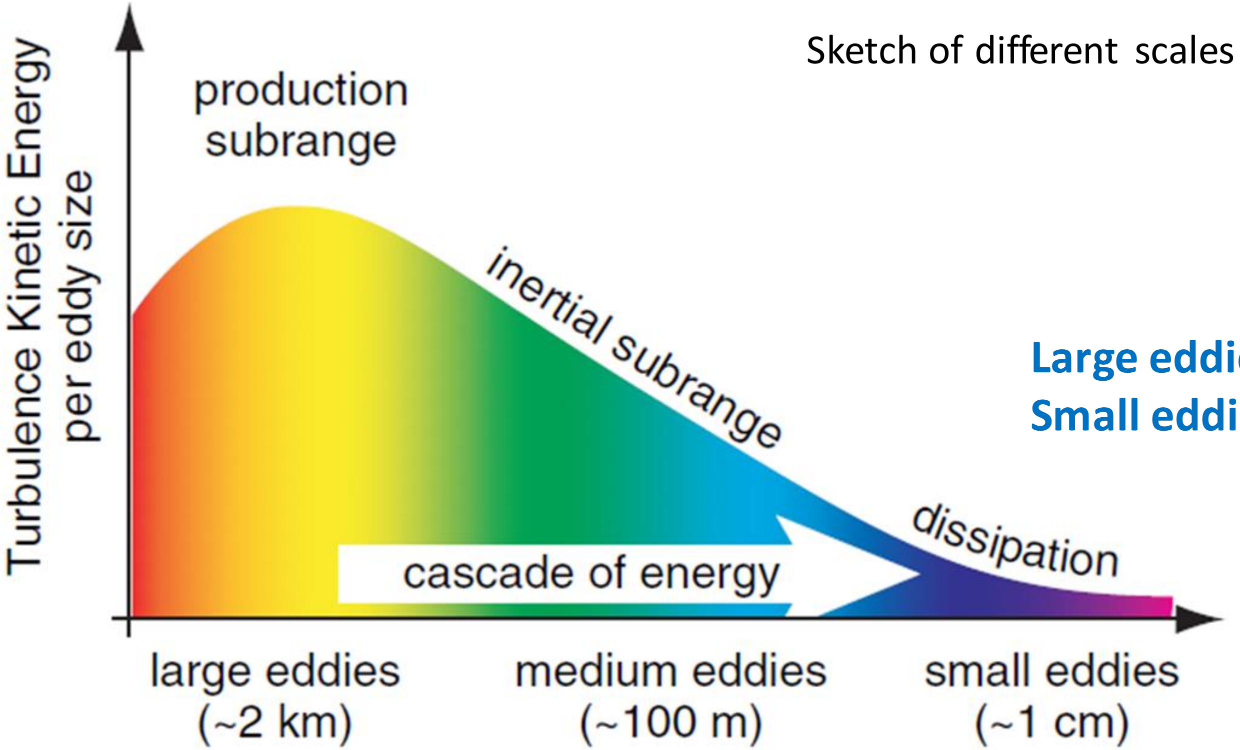
Scientific questions

- What is the feedback mechanism between the aerosol radiation effect and the atmospheric boundary layer under the heavy smoggy conditions?
- Will the classical atmospheric turbulence be turned into intermittent turbulence with the persistent existence of smog?
- Is the Monin-Obukhov Similarity Theory suitable for surface layer of the smoggy boundary layer?

Introduction of LES



Sketch of different scales of turbulent eddies in the PBL(from Baidu)



Large eddies: solving N-S equation directly
Small eddies: parameterization

The spectrum of turbulence kinetic energy (Source: Courtesy of Roland B. Stull)

LES equations

N-S equations for the resolvable wind fields

$$\frac{\partial \bar{u}}{\partial t} = \overline{\overline{v\zeta_z}} - \overline{\overline{w\zeta_y}} + f\bar{v} - \frac{\partial P^*}{\partial x} - \frac{\partial \langle \bar{p} \rangle}{\partial x} - \frac{\partial \tau_{xx}}{\partial x} - \frac{\partial \tau_{xy}}{\partial y} - \frac{\partial \tau_{xz}}{\partial z}$$

$$\frac{\partial \bar{v}}{\partial t} = \overline{\overline{w\zeta_x}} - \overline{\overline{u\zeta_z}} - f\bar{u} - \frac{\partial P^*}{\partial y} - \frac{\partial \langle \bar{p} \rangle}{\partial y} - \frac{\partial \tau_{xy}}{\partial x} - \frac{\partial \tau_{yy}}{\partial y} - \frac{\partial \tau_{yz}}{\partial z}$$

$$\frac{\partial \bar{w}}{\partial t} = \overline{\overline{u\zeta_y}} - \overline{\overline{v\zeta_x}} + \frac{g\bar{\theta}}{\theta_0} - \frac{\partial P^*}{\partial z} - \frac{\partial \tau_{xz}}{\partial x} - \frac{\partial \tau_{yz}}{\partial y} - \frac{\partial \tau_{zz}}{\partial z} - \left\langle \overline{\overline{u\zeta_y}} - \overline{\overline{v\zeta_x}} + \frac{g\bar{\theta}}{\theta_0} - \frac{\partial P^*}{\partial z} - \frac{\partial \tau_{xz}}{\partial x} - \frac{\partial \tau_{yz}}{\partial y} - \frac{\partial \tau_{zz}}{\partial z} \right\rangle$$

$$\nabla^2 P^* = \frac{\partial H_x}{\partial x} + \frac{\partial H_y}{\partial y} + \frac{\partial H_z}{\partial z}$$

Poisson equation for pressure to enforce incompressibility

Equation for thermal field

$$\frac{\partial \bar{\theta}}{\partial t} = -\overline{\bar{u}\frac{\partial \bar{\theta}}{\partial x}} - \overline{\bar{v}\frac{\partial \bar{\theta}}{\partial y}} - \overline{\bar{w}\frac{\partial \bar{\theta}}{\partial z}} - \frac{\partial \tau_{\theta x}}{\partial x} - \frac{\partial \tau_{\theta y}}{\partial y} - \frac{\partial \tau_{\theta z}}{\partial z}$$

SGS TKE

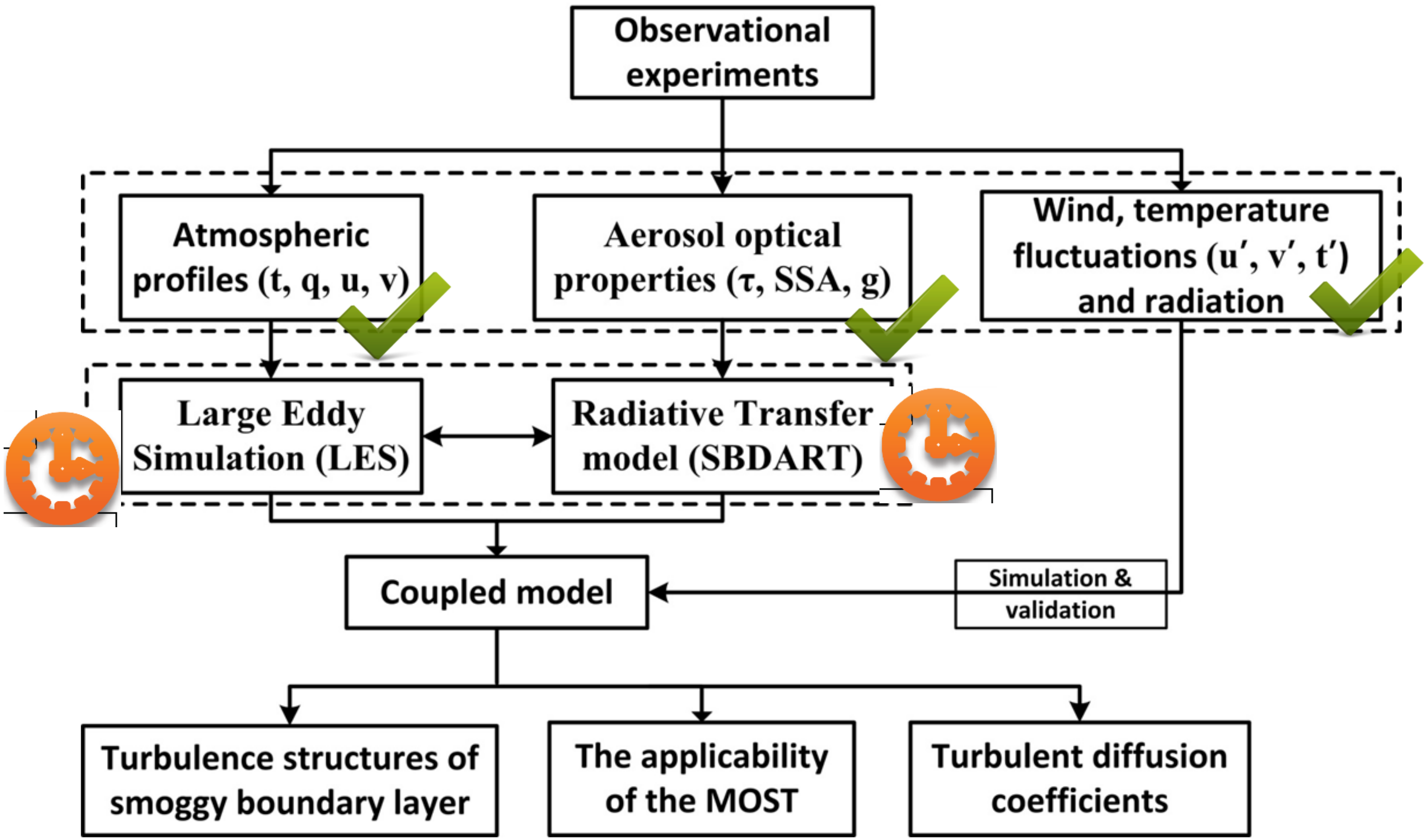
$$\frac{\partial \bar{e}'}{\partial t} = -\overline{\bar{u}_i \frac{\partial \bar{e}'}{\partial x_i}} - \overline{u_i' u_j'} \frac{\partial \bar{u}_i}{\partial x_j} + \frac{g}{\theta_0} \overline{w'\theta'} - \frac{\partial \left[\overline{u_i'(e' + p'/\rho_0)} \right]}{\partial x_i} - \varepsilon$$

$$\tau_{ij} = -K_M \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)$$

$$\tau_{\theta i} = -K_H \frac{\partial \bar{\theta}}{\partial x_i}$$

The SGS fluxes are related to the resolved-scale field as

Method: Technology roadmap

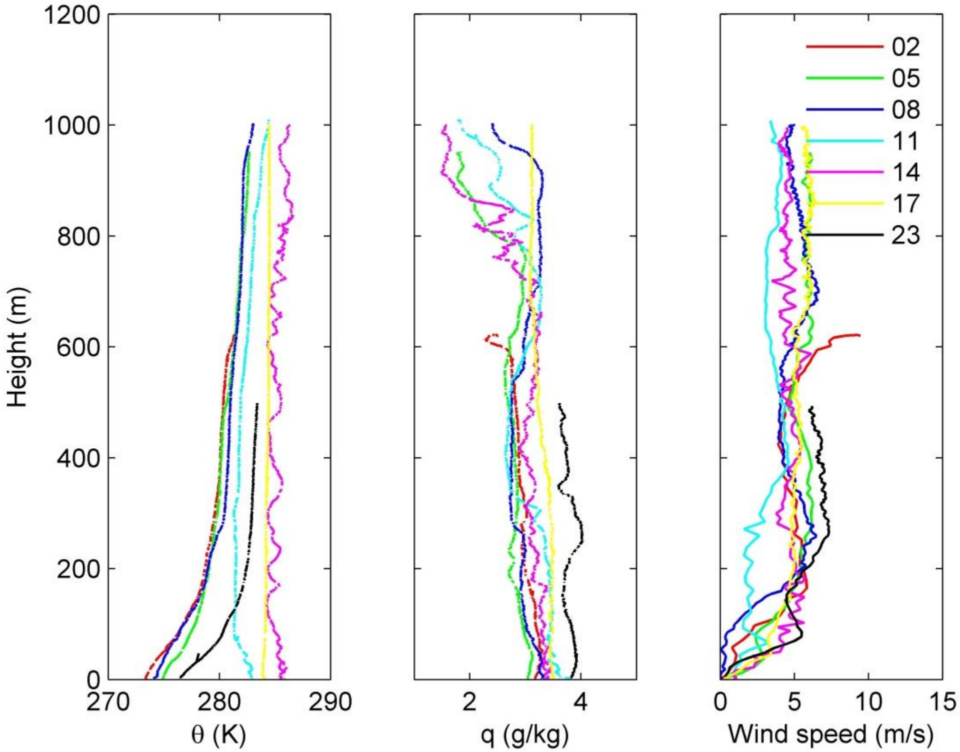


A summary of field experiments in January 2015

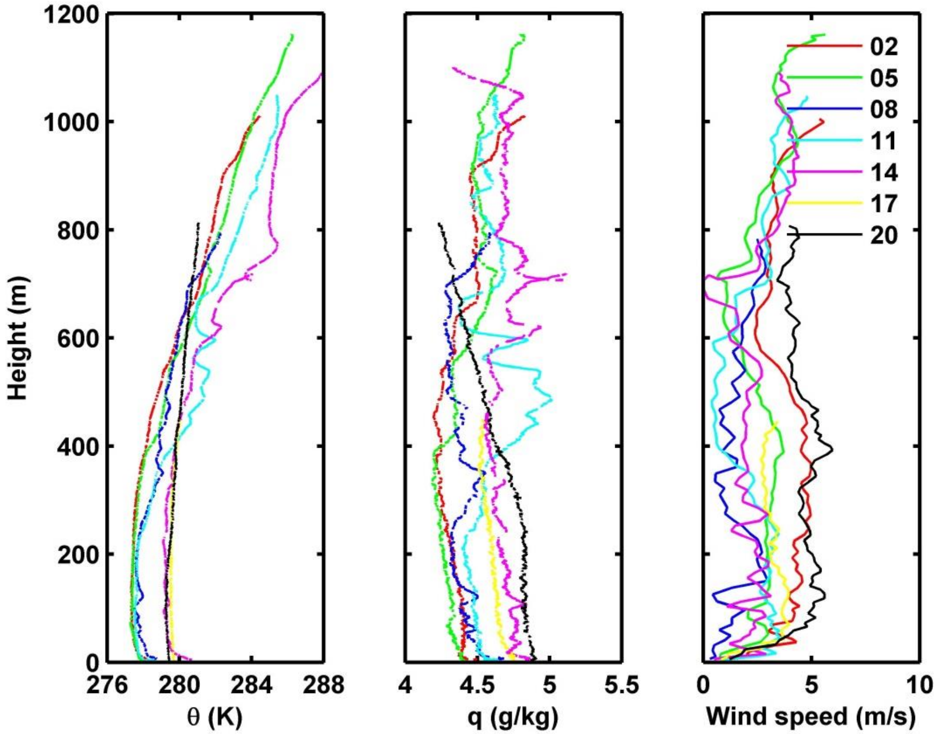
	2:00	5:00	8:00	11:00	14:00	17:00	20:00	23:00	AQI
2015/1/9	622	950	1000	1008	1000	1000	No	498	164
2015/1/10	870	360	1000	1000	970	980	170	200	159
2015/1/11	130	150	900	1000	1100	360	No	No	170
2015/1/12	No	No	No	No	No	No	No	No	70
2015/1/13	No	No	No	No	No	No	No	No	68
2015/1/14	No	No	No	No	730	800	1000	930	52
2015/1/15	800	800	525	1000	1000	1000	No	1000	67
2015/1/16	990	890	450	610	100	380	140	70	134
2015/1/17	70	400	490	980	1010	740	50	No	134
2015/1/18	No	No	330	No	No	No	100	80	107
2015/1/19	100	190	860	1000	1000	720	90	250	117
2015/1/20	50	No	No	No	No	No	720	450	109
2015/1/21	340	No	No	No	No	No	No	No	159
2015/1/22	No	No	1000	1000	1000	1100	1000	1000	157
2015/1/23	1000	220	250	490	930	840	40	260	165
2015/1/24	1000	270	1000	240	290	140	No	310	240
2015/1/25	90	No	No	No	No	No	1000	1000	234
2015/1/26	1000	1100	790	1000	1000	449	810	No	281

Lifting height of tethered balloon during the boundary layer profile observation experiment in January, 2015 at NUIST site (shaded areas represent the days with relatively complete data.).

Observed vertical profiles on two different haze days



Vertical profiles of potential temperature (θ), specific humidity (q), and wind speed on 9th January



The same as the left, but for 26th January

Configuration of the LES

- Domain size: 6.4km x 6.4km x 2.56km
- Grid numbers: 128 x 128 x 128
- Grid spacing: 50m x 50m x 20m

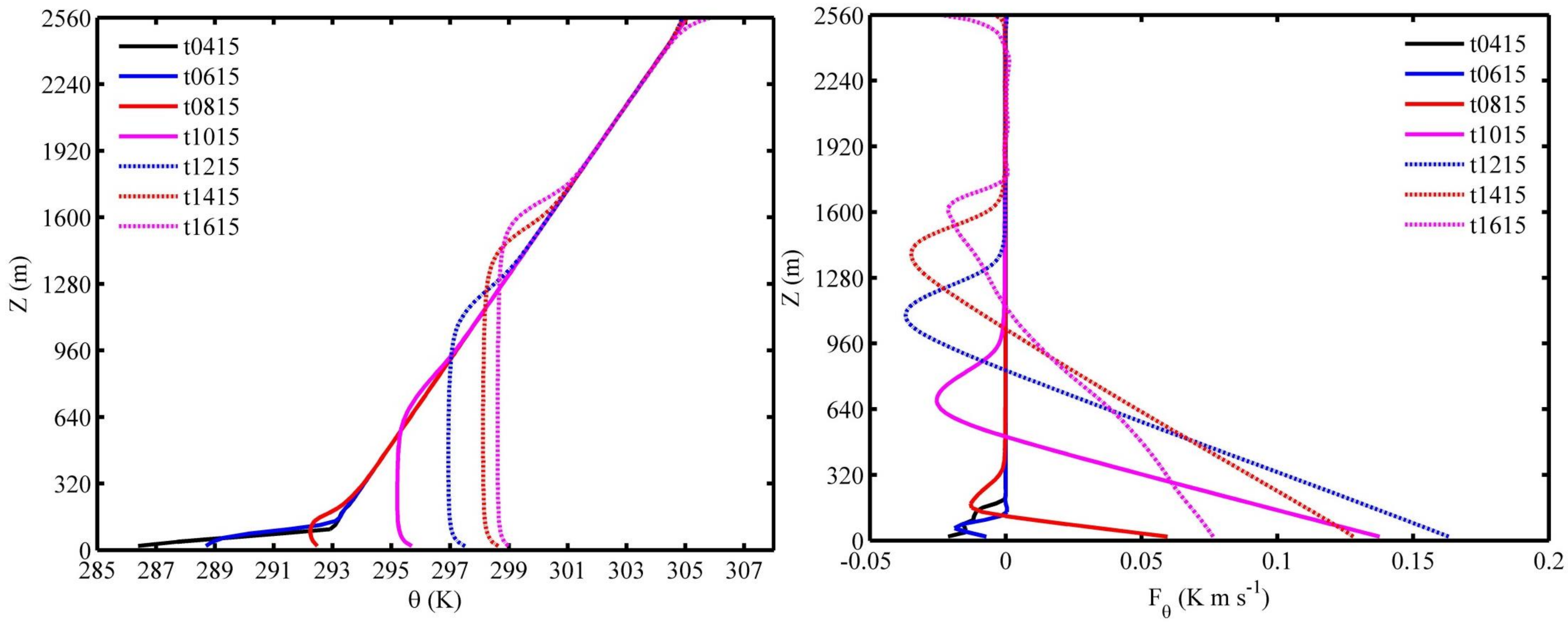
Domain setup

- Simulated time: from 04:15 to 16:15 (LST)

20,000 time step;
Spend around 9.5 h

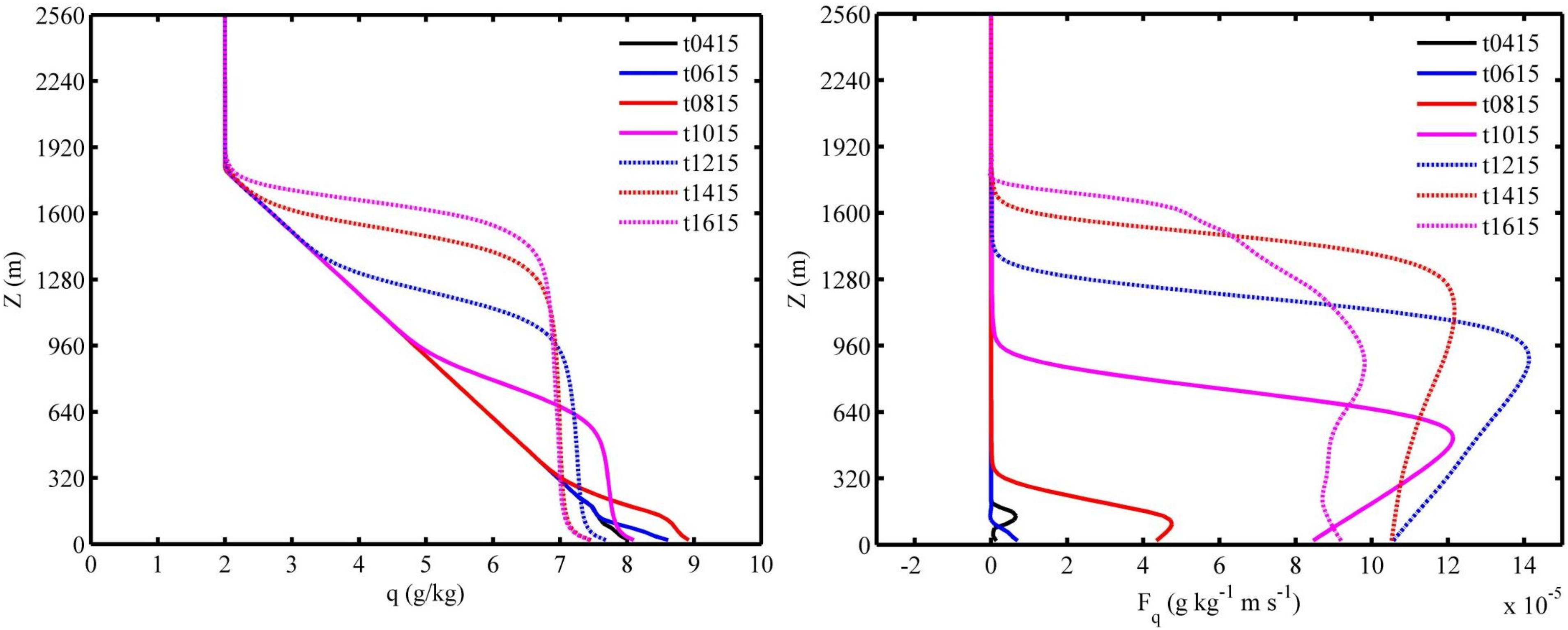
- Initial conditions: θ and q profiles adopted from 1994 intensive field campaigns in the BOREAS (*Huang et al., 2011*).
- Boundary conditions and numerical schemes follow Huang's setup.

LES preliminary results



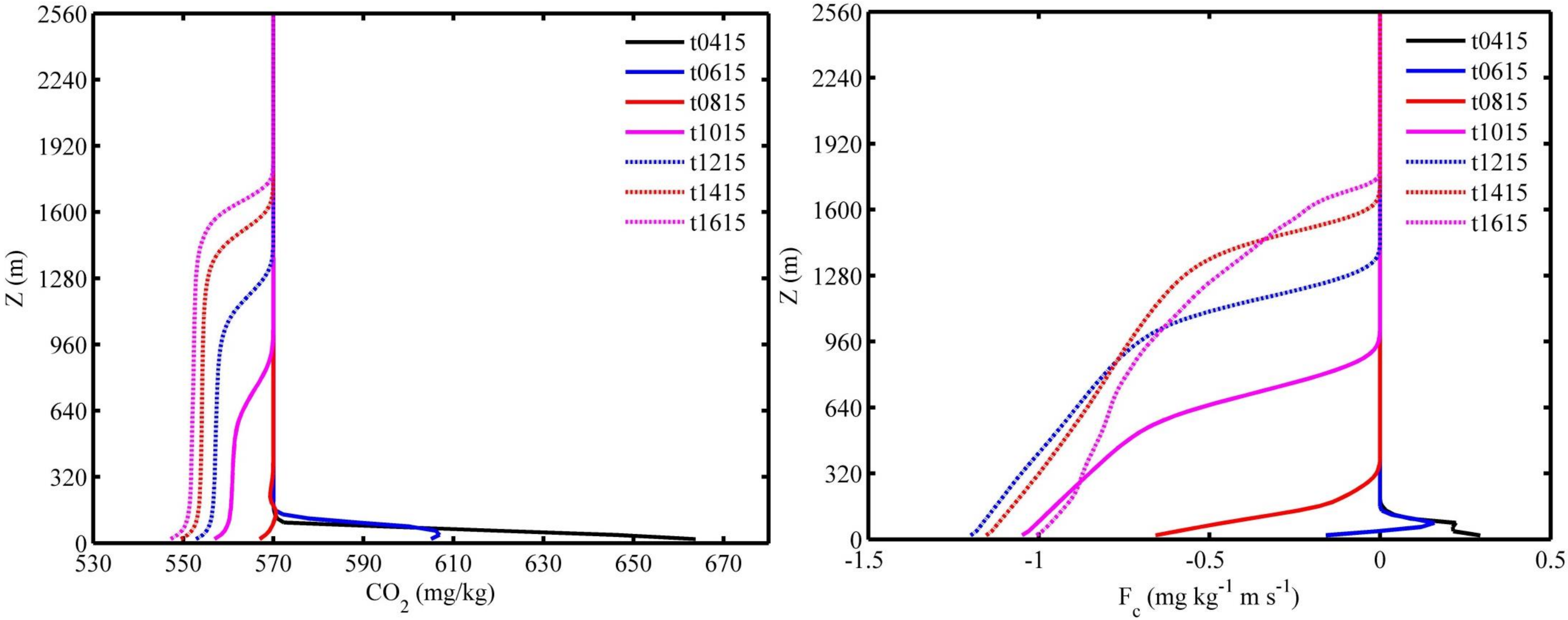
Vertical profiles of potential temperature (θ) and heat flux (F_θ) at u_g = 5 m/s

LES preliminary results (cont.)



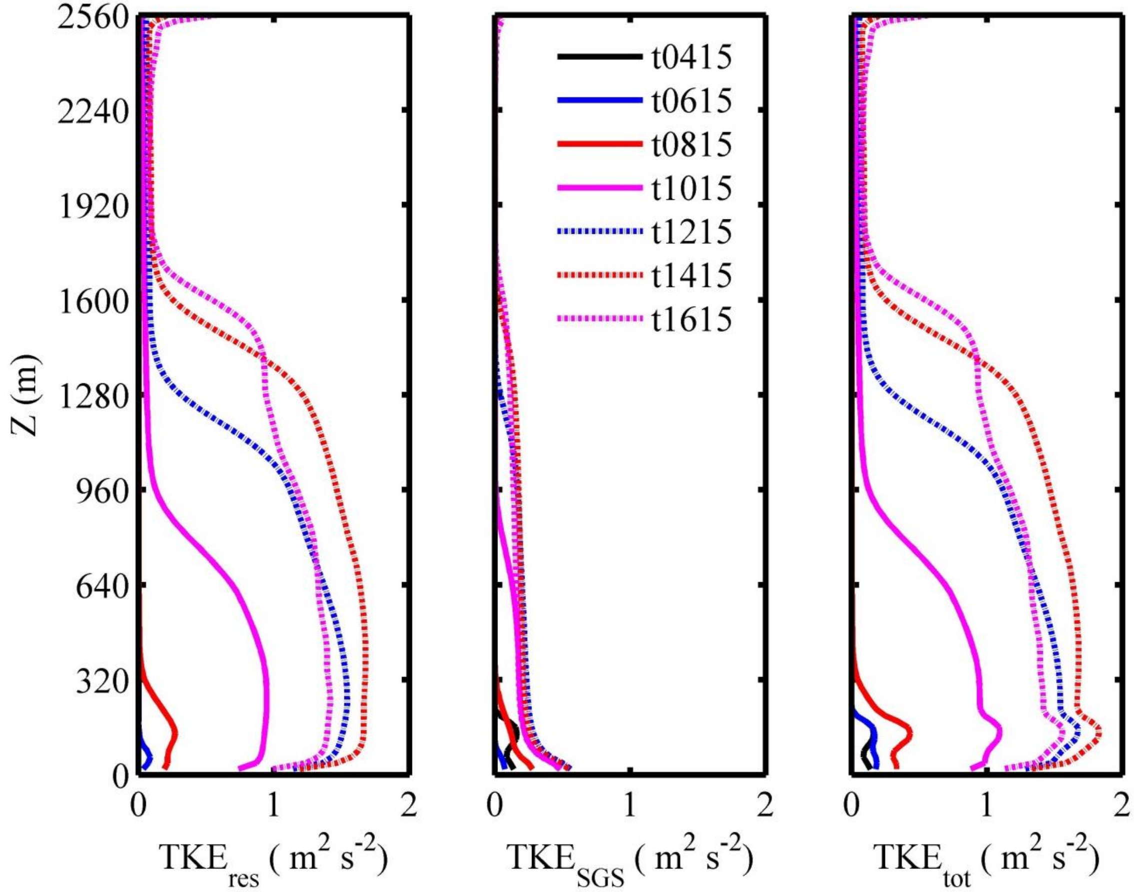
Vertical profiles of specific humidity (q) and specific humidity flux (F_q) at u_g = 5 m/s.

LES preliminary results (cont.)



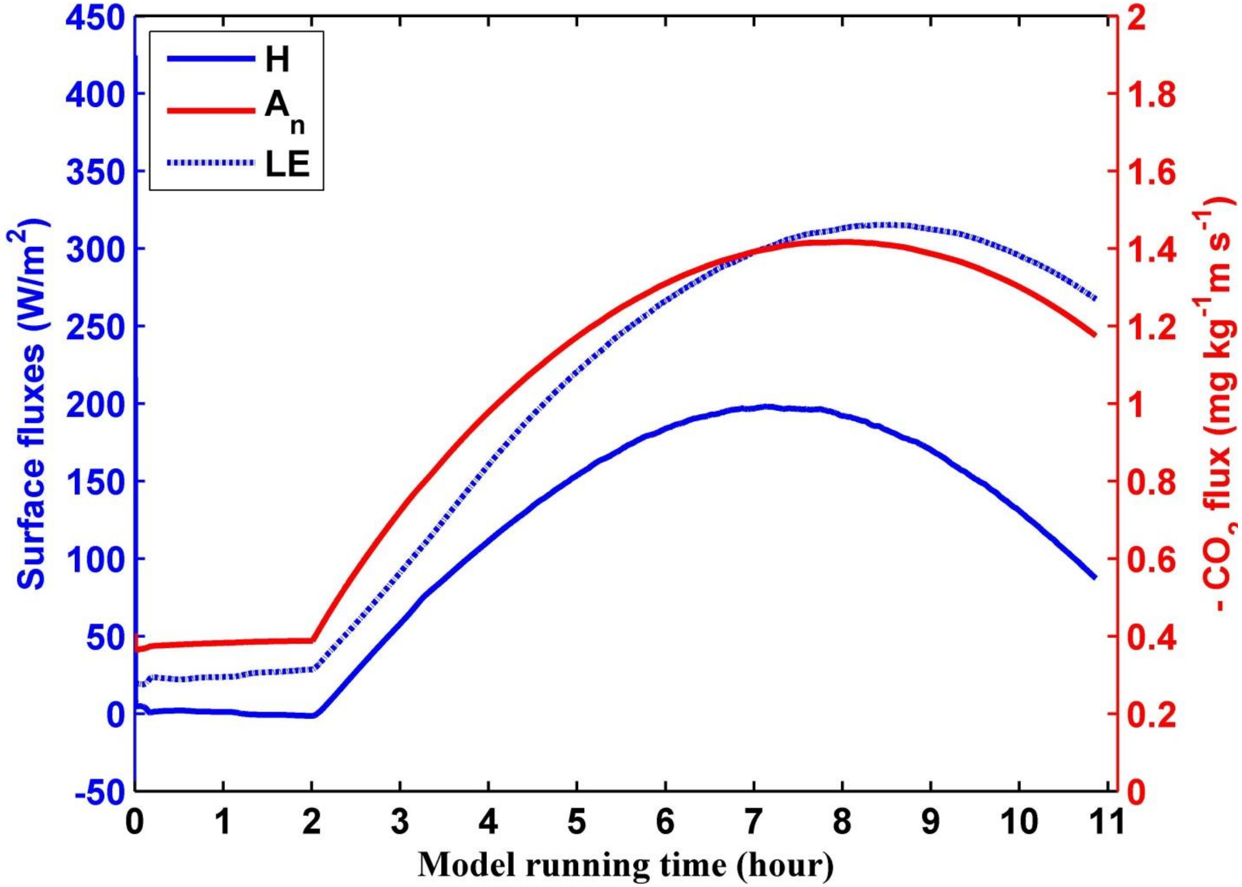
Vertical profiles of CO_2 mixing ratio (c) and CO_2 flux (F_c) at u_g = 5 m/s.

LES preliminary results (cont.)



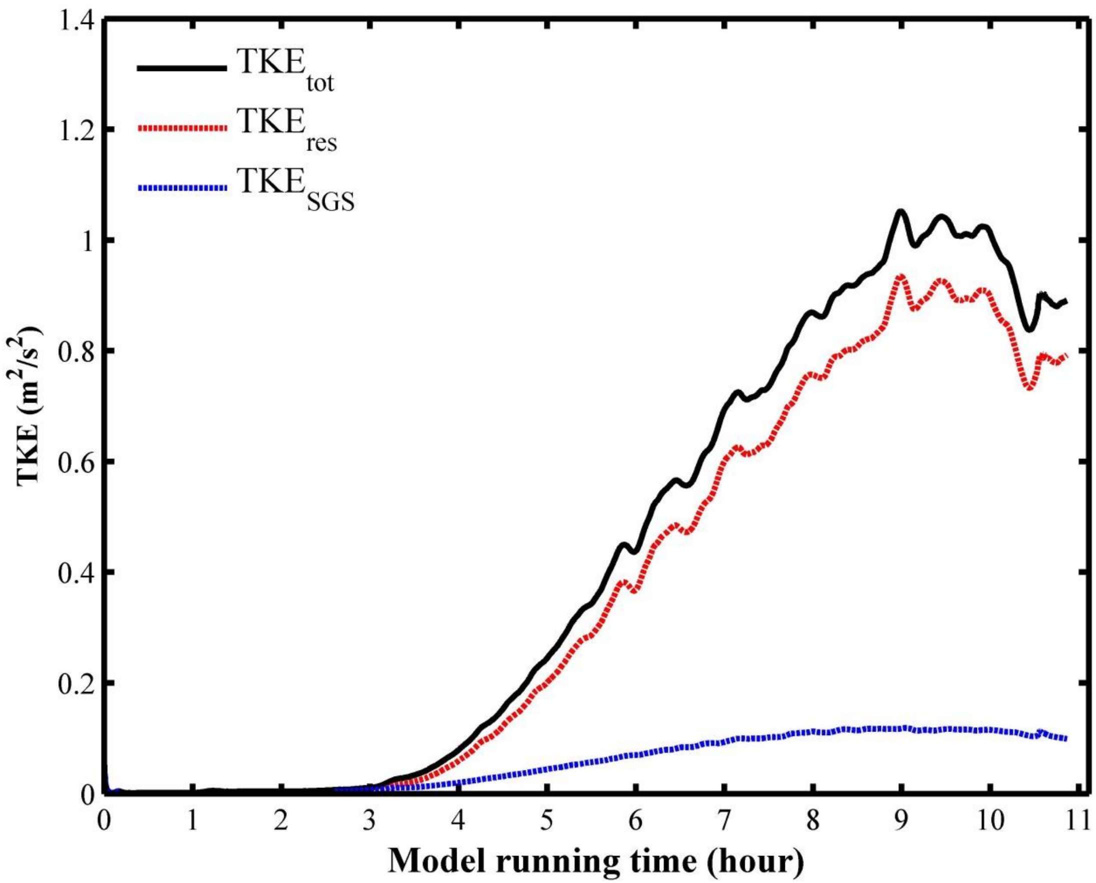
Vertical profiles of turbulent kinetic energy of the resolvable-scale field, subgrid-scale field and total field.

LES preliminary results (cont.)



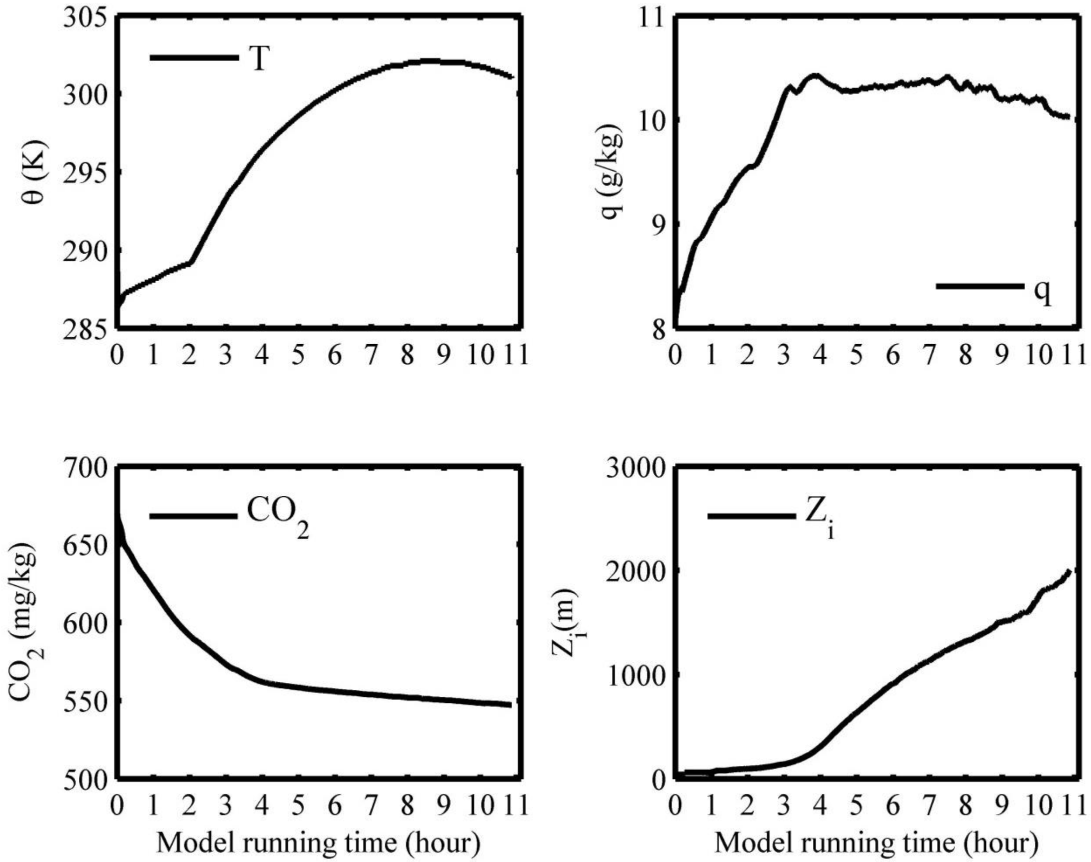
Temporal variations in sensible heat flux (H), latent heat flux (LE), and CO_2 flux (An) averaged across the whole domain at u_g=5m/s.

LES preliminary results (cont.)



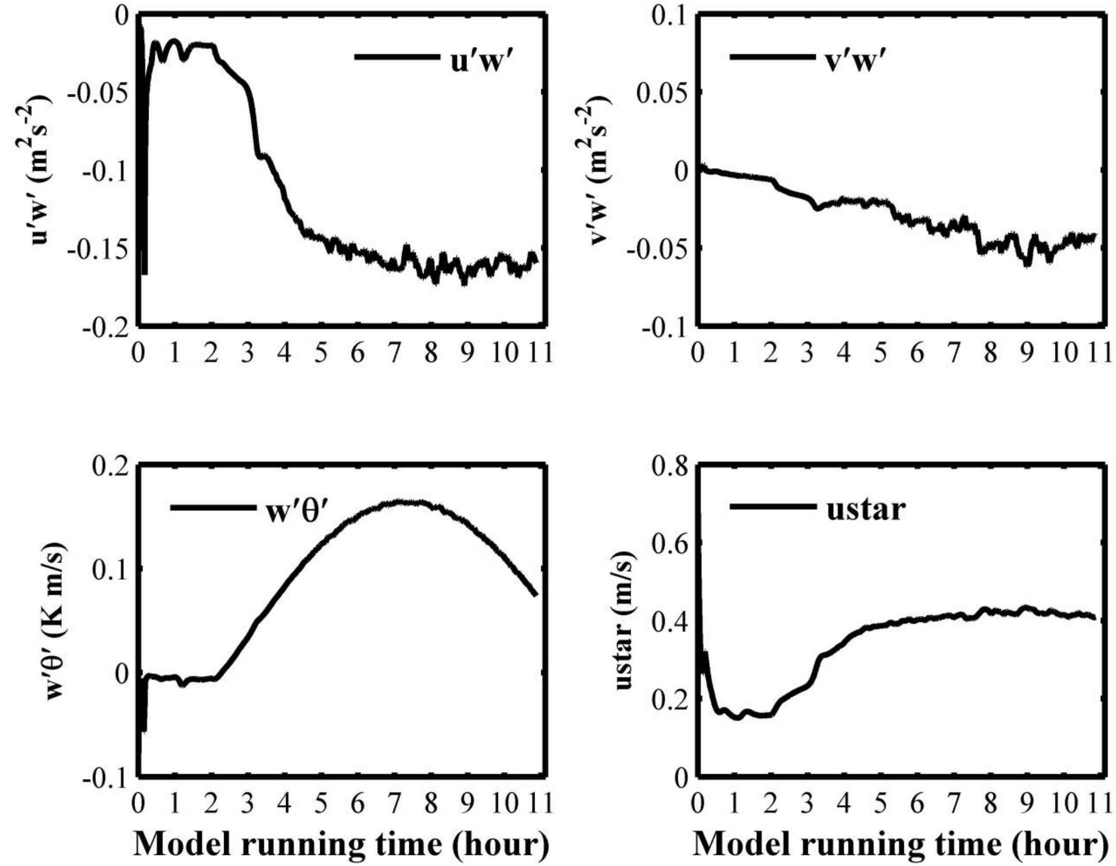
Temporal variations of turbulent kinetic energy of the resolvable-scale field, subgrid-scale field and total field.

LES preliminary results (cont.)



Temporal variations of potential temperature (θ), specific humidity (q), CO_2 mixing ratio, and the mixed-layer height (Z_i).

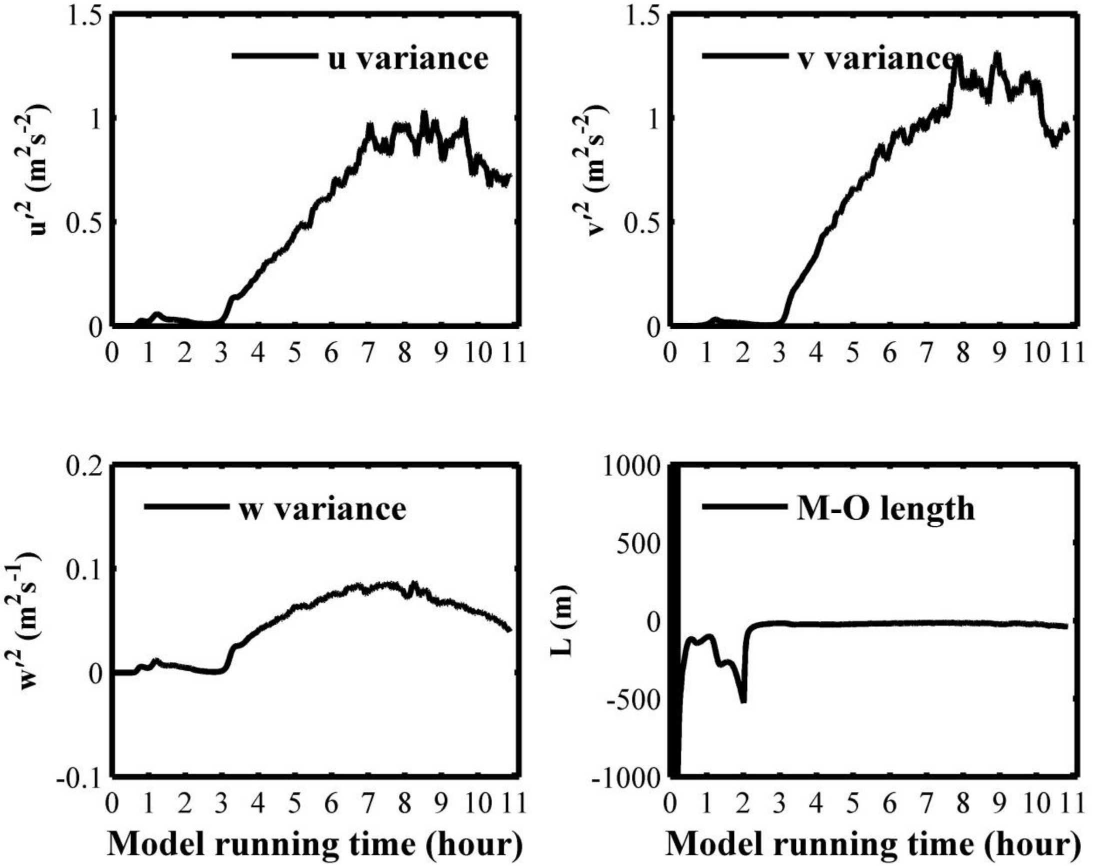
LES preliminary results (cont.)



$$u^* = [(\overline{u'w'})^2 + (\overline{v'w'})^2]^{1/4}$$

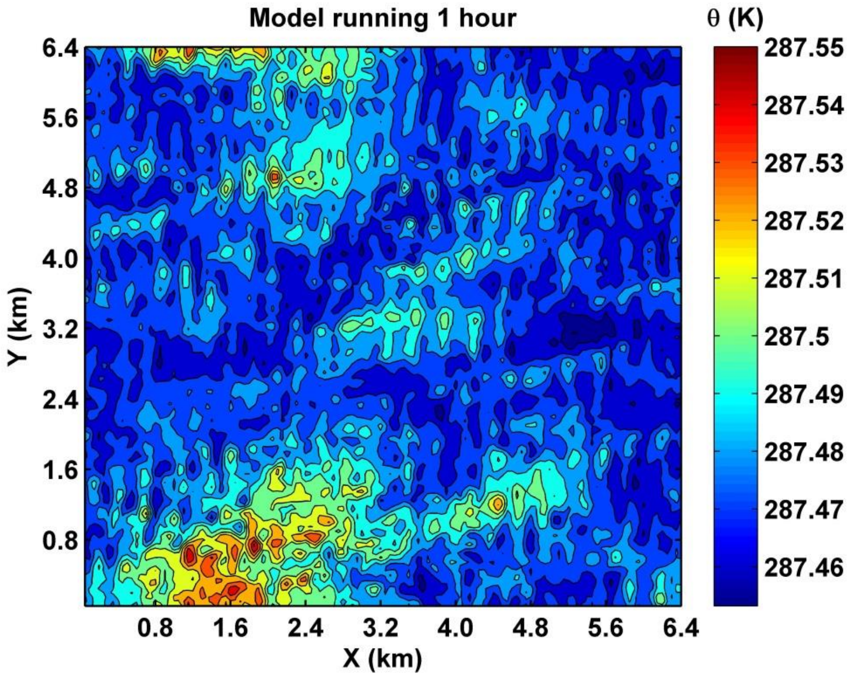
Temporal variations of $\overline{u'w'}$ flux, $\overline{v'w'}$ flux, $\overline{w'\theta'}$ flux and friction velocity (u*).

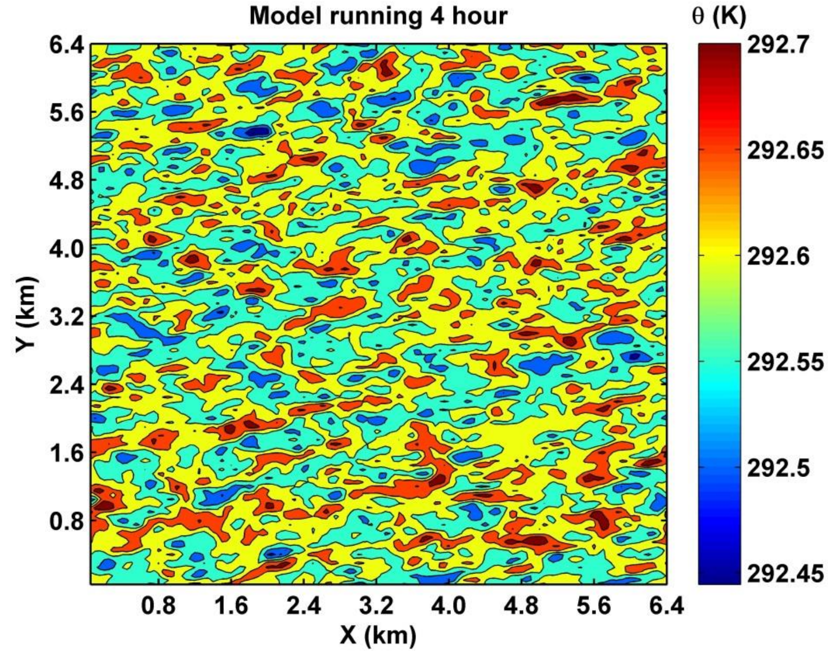
LES preliminary results (cont.)



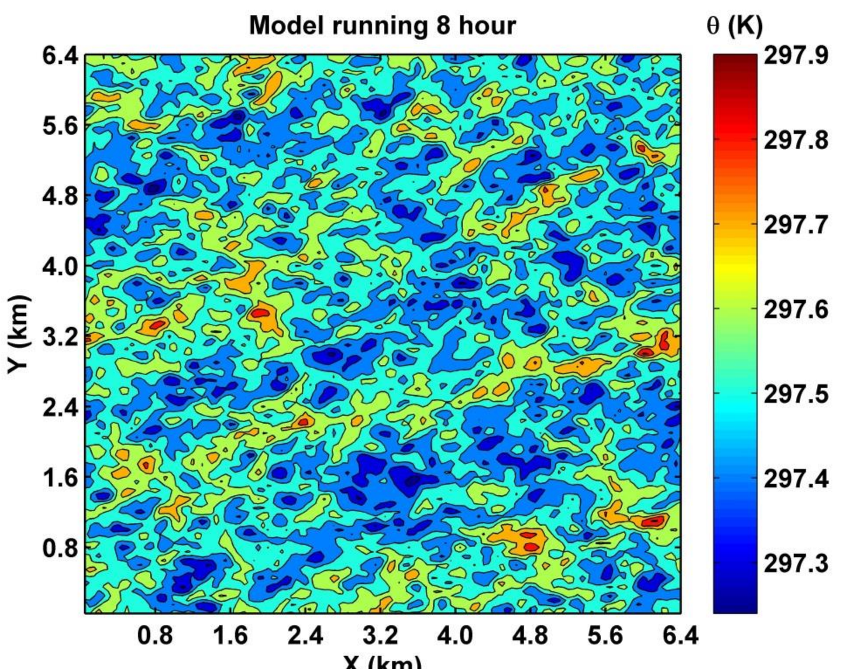
L>0, stable
L<0, unstable
$|\mathbf{L}| \rightarrow \infty$, neutral

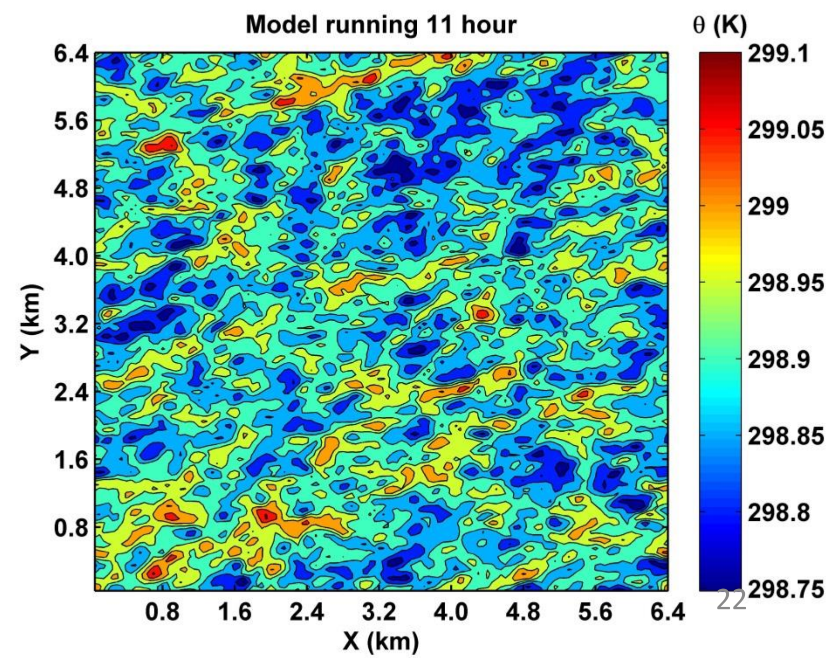
Temporal variations of $\overline{u'^2}$, $\overline{v'^2}$, $\overline{w'^2}$ and M-O length (L).

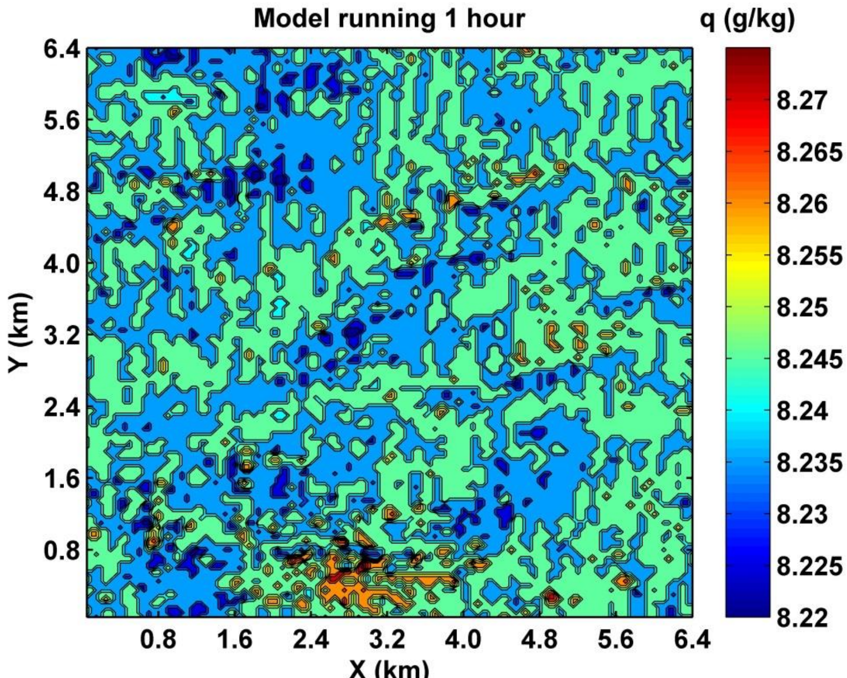


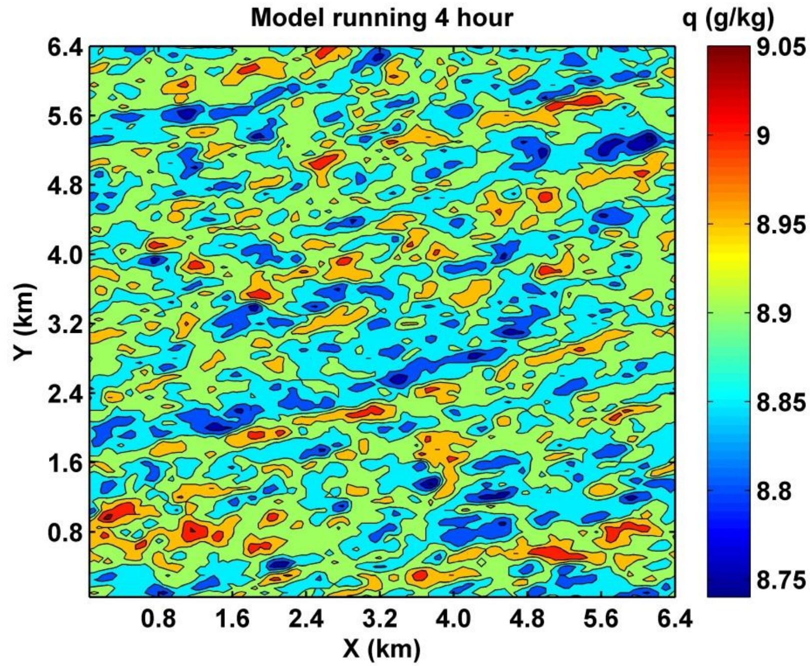


Hourly-averaged surface fields of potential temperature for different time.

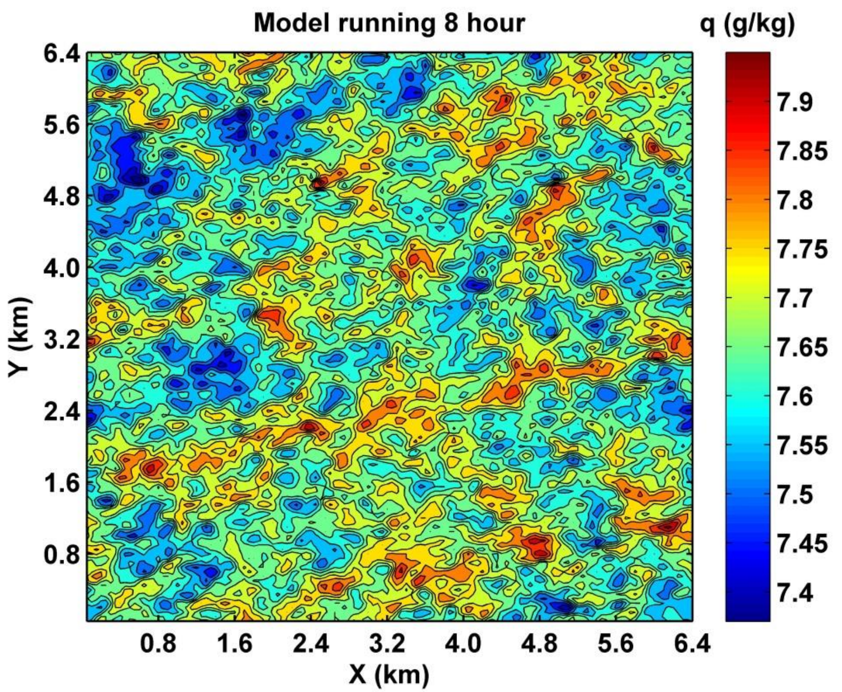


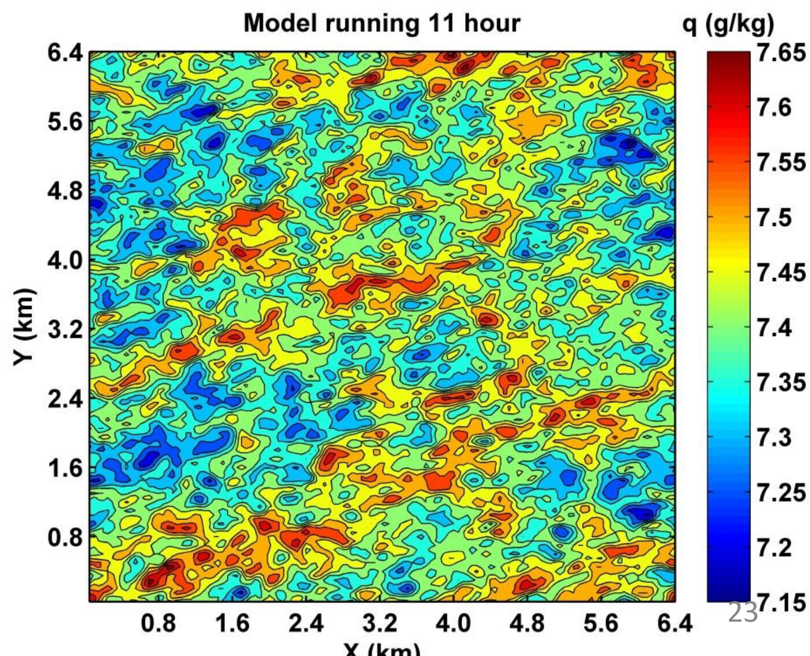


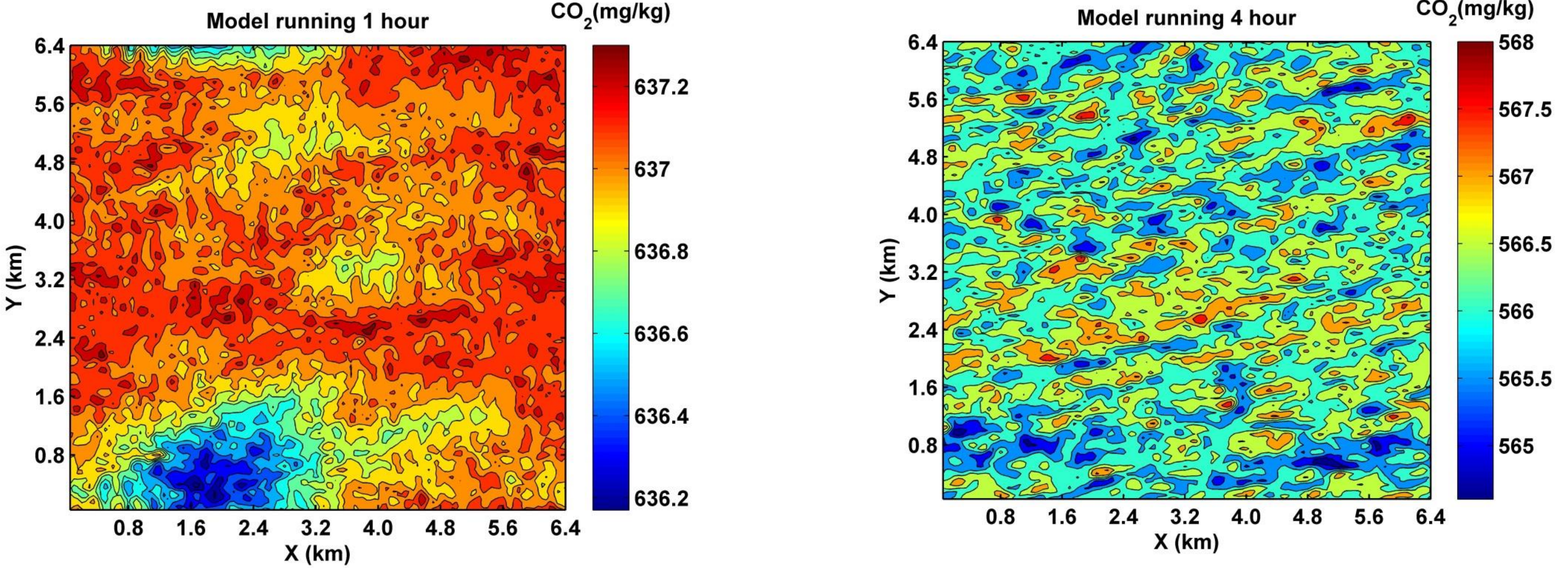




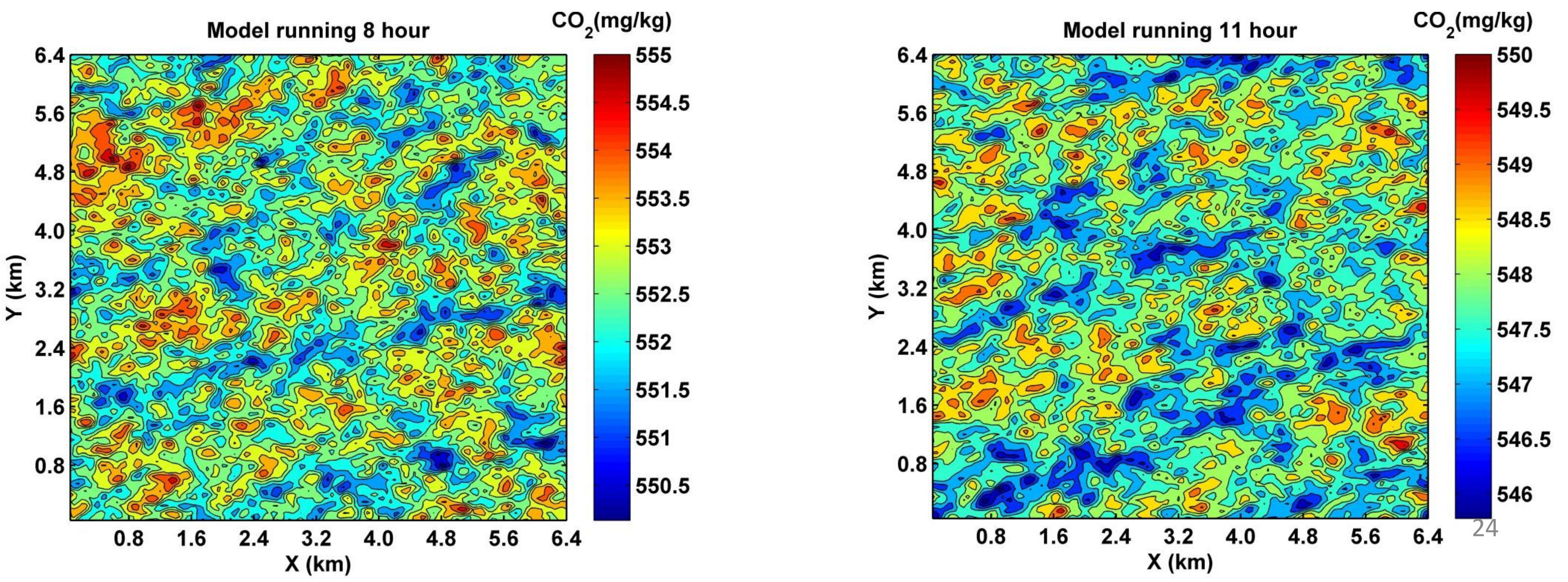
Hourly-averaged surface fields of water vapor for different time.







Hourly-averaged surface fields of CO_2 concentration for different time.



Summary

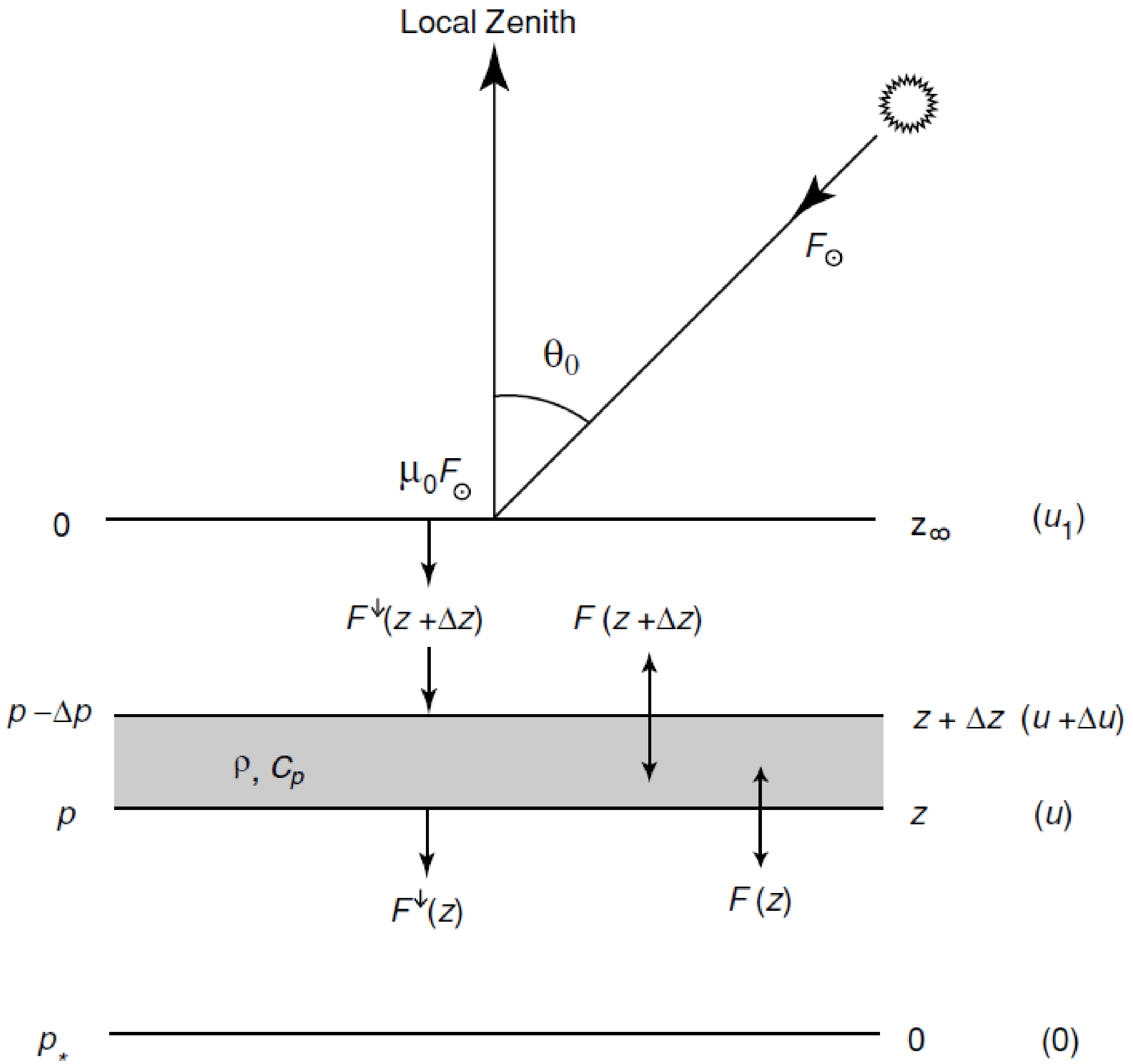
- The LES model was run on NUIST super computer successfully.

- The LES simulations show similar results to Huang et al. (2011)

On-going work

- A case study: detailed comparison of LES model results with the observations (vertical profiles).
- Offline testing of the atmospheric radiation transfer model (SBDART) for calculating the heating rate at different heights on a heavy smoggy day.
- Include the calculated atmospheric heating rate in the LES model to assess the impact of the aerosol radiation effect on the smoggy boundary layer structure.

Fundamental



$$\Delta F(z) = F(z) - F(z+\Delta z).$$

$$\Delta F(z) = -\rho C_p \Delta z \frac{\partial T}{\partial t}.$$

$$\frac{\partial T}{\partial t} = -\frac{1}{\rho C_p}\frac{\Delta F(z)}{\Delta z} = \frac{g}{C_p}\frac{\Delta F(p)}{\Delta p} = -\frac{q}{C_p}\frac{\Delta F(u)}{\Delta u}$$

$$dp = -\rho g\, dz,$$

μ_0 solar zenith angle

$F_\odot$ the solar spectral irradiance

(Liou et al., 2002)

Thank You !