Update on large eddy simulation of boundary layer with aerosol radiative heating

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Introduction

- Entrainment is critical to the development of the ABL and provides a constraint on exchange of energy and species between the free atmosphere and the ABL.
- Quantification of entrainment represents one of the most challenge problems in the modeling of the ABL. Entrainment isn't well known due to scarcity of observational data and high-resolution simulations.
- Entrainment rate normalized with convective velocity shows -1 law with Richardson number (*Ri*) at low *Ri* (<10) but -3/2 law at high *Ri* (>10.0) in the clean ABL.
- The sensible heat flux follows linear relationship with height for the clean ABL.

Objectives

- A radiation transfer model is coupled with a large-eddy simulation (LES) model to investigate the impact of aerosol radiative effect on the thermodynamics and entrainment of the ABL.
- **Specific Objectives**
  - Derivation and evaluation of entrainment rate equation by including the aerosol radiative effect.
  - Determination of relationship of sensible heat flux with height.
  - Investigation of how aerosol radiative heating changes entrainment flux ratio.

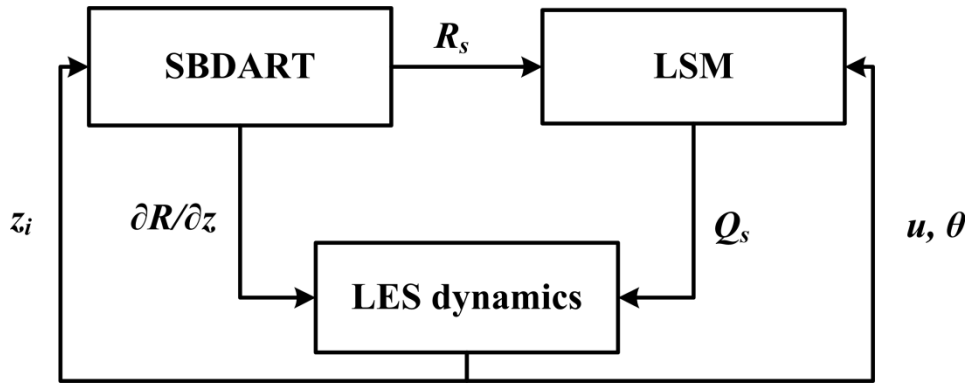
Model

- LES in this study was originally developed by *Moeng (1984)*, and refined by *Sullivan (1996)*, *Patton et al. (2005)* and *Huang et al. (2008, 2009, and 2011)*.

- Governing equation of θ :

$$\frac{\partial \theta}{\partial t} = -u\frac{\partial \theta}{\partial x} - v\frac{\partial \theta}{\partial y} - w\frac{\partial \theta}{\partial z} - \frac{\partial \tau_{\theta x}}{\partial x} - \frac{\partial \tau_{\theta y}}{\partial y} - \frac{\partial \tau_{\theta z}}{\partial z} + \boxed{\frac{\partial R}{\partial z}}$$

- The Santa Barbara Discrete Ordinates Radiative Transfer (DISORT) Atmospheric Radiative Transfer model (SBDART)
  - Input parameters (aerosol optical property parameters): *AOD*, *SSA*, and *g*.
  - Output: heating rate, R_s



Numerical Experiments

	$d\theta/dz$=3 K km^{-1}	$d\theta/dz$=6 K km^{-1}	$d\theta/dz$=9 K km^{-1}
CTL	CTLN3	CTLN6	CTLN9
AOD=0.3	A03N3	A03N6	A03N9
AOD=0.6	A06N3	A06N6	A06N9
AOD=0.9	A09N3	A09N6	A09N9
AOD=1.2	A12N3	A12N6	A12N9
AOD=1.5	A15N3	A15N6	A15N9

Domain size is 5 km × 5 km × 1.92 km with grid spacing of 50 m × 50 m × 20 m in the x, y, and z directions, respectively. (SSA=0.9, and g=0.6)

Profiles of potential temperature

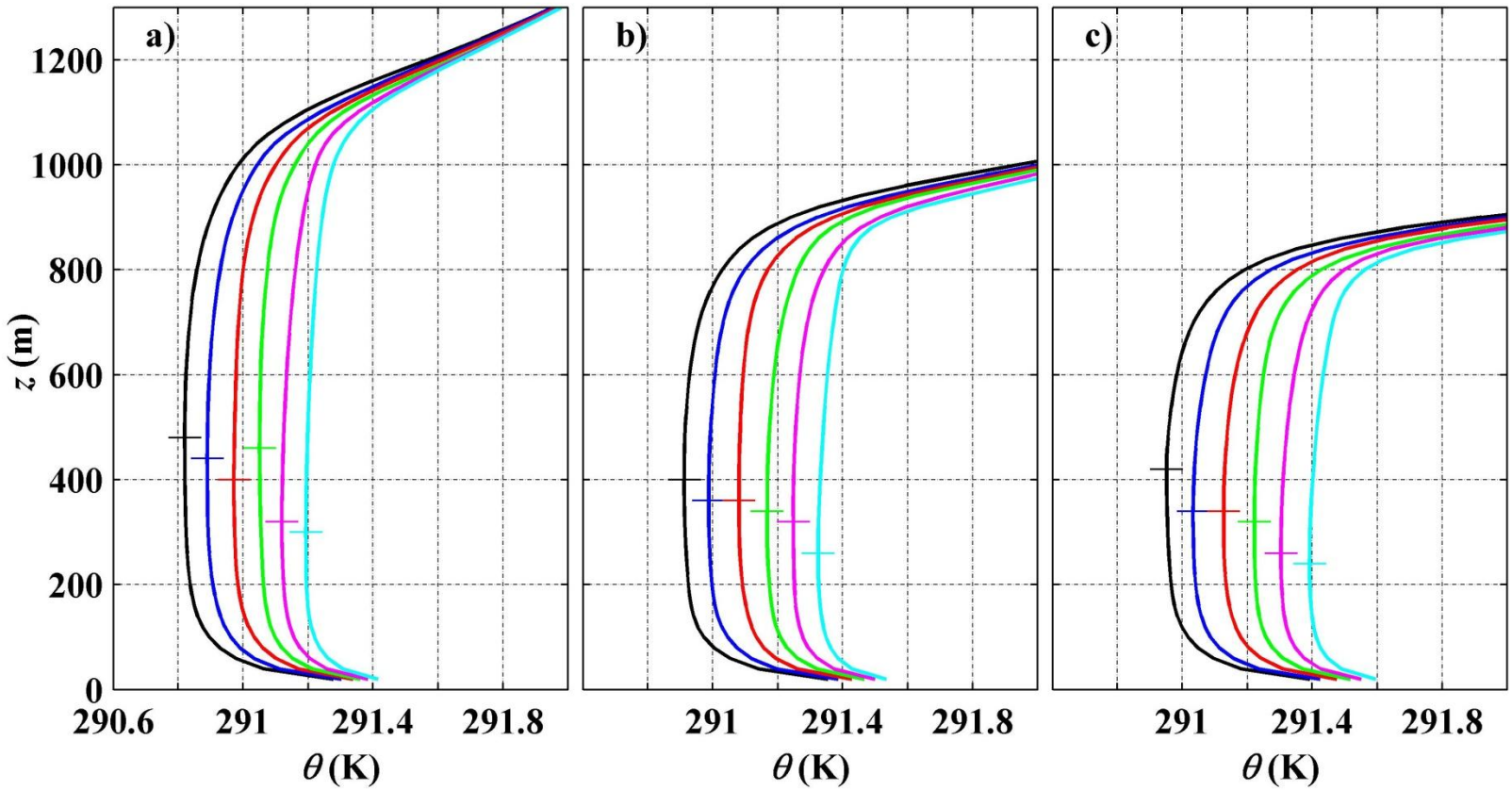


Figure 1. Profiles of temperature under a) dθ/dz=3 K km^{-1}, b) dθ/dz=6 K km^{-1}, c) dθ/dz=9 K km^{-1}. Black: CTL, blue: A03, red: A06, green: A09, magenta: A12, cyan: A15. The short dash represents the position of dθ/dz=0.

Temperature profile from WRF-Chem

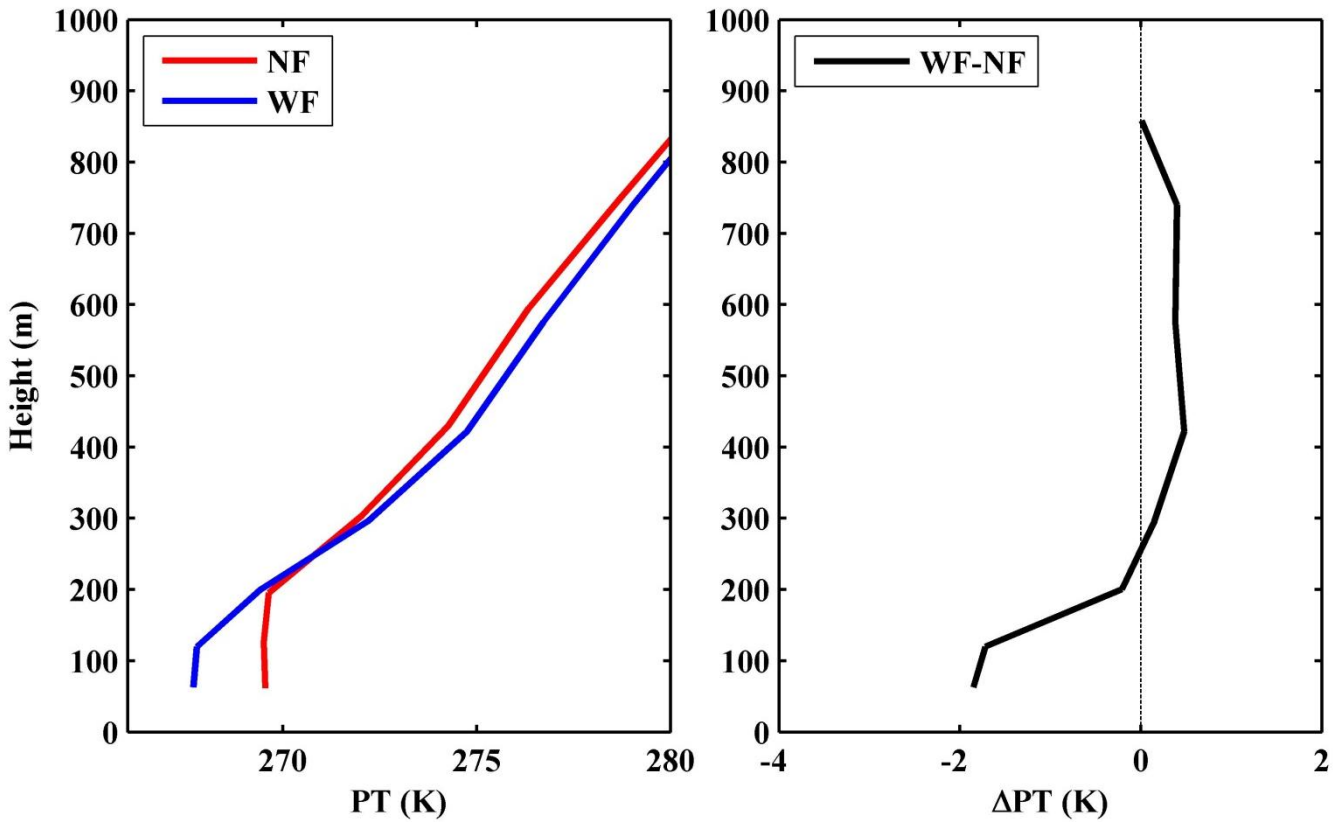


Figure 2. Potential temperature profile (left) and the difference (right) between aerosol case and non-aerosol case at 13:00pm LST. *Data from Meng Gao (Harvard University).*

Profiles of turbulence heat flux and radiation flux

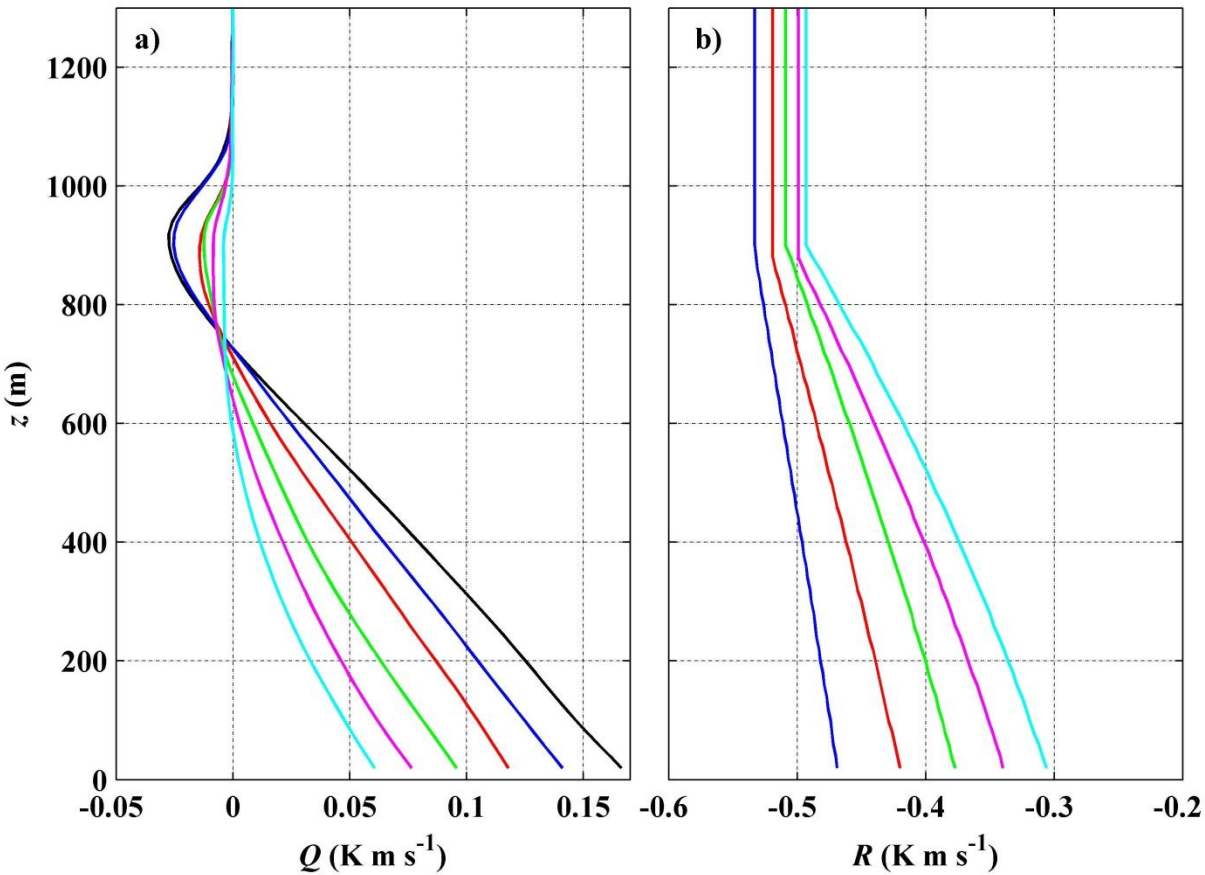


Figure 3. Profiles of a) turbulence heat flux and b) radiation flux under dθ/dz=6 K km^{-1}. Black: CTL, blue: A03, red: A06, green: A09, magenta: A12, cyan: A15.

Proposed new zero-order model framework

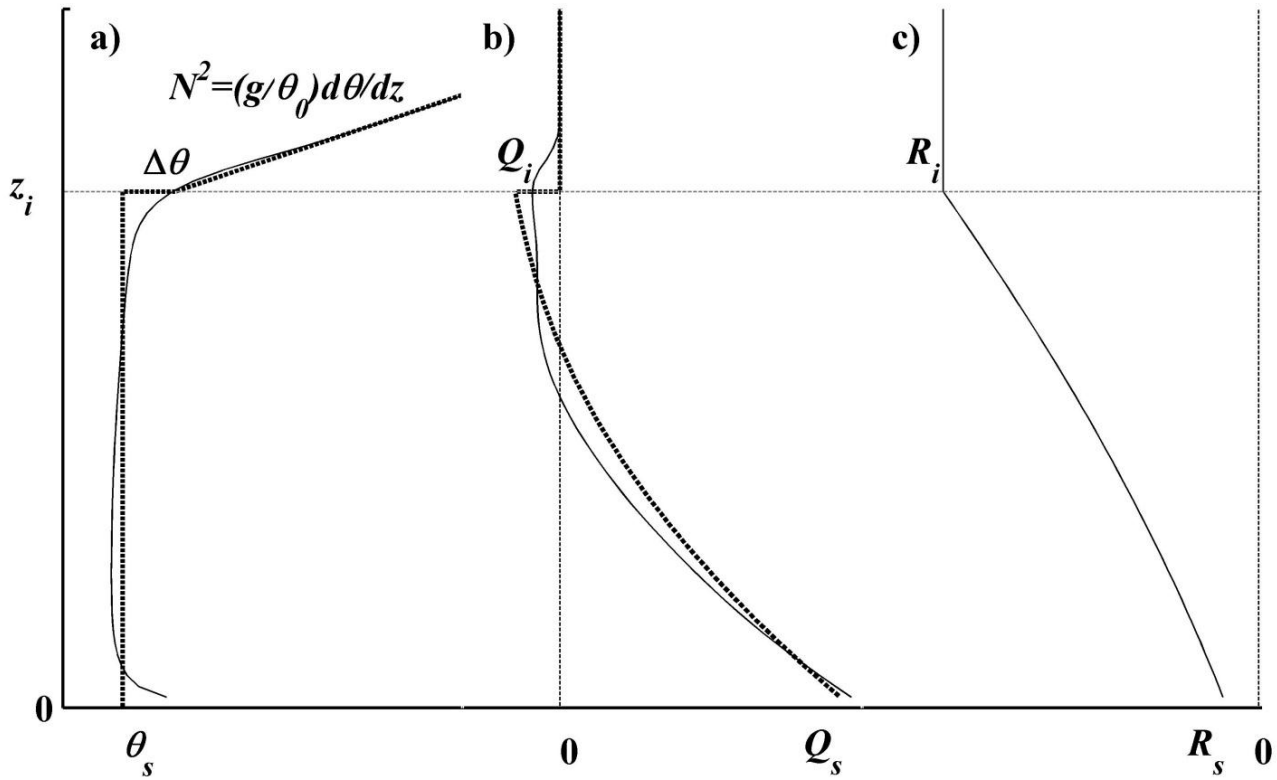


Figure 4. Profiles of a) temperature, b) turbulence heat flux and c) radiation flux in ZOM framework. Thin solid lines indicate LES profiles and heavy dash lines are their ZOM counterparts.

Derivation of entrainment equation

- Governing equation of potential temperature in the ABL with aerosols:

$$\frac{\partial \theta}{\partial t} = -\frac{\partial Q}{\partial z} - \frac{\partial R}{\partial z}, \qquad (1)$$

- After taking integral (1) from 0 to $z \le z_i$

$$Q(z) + R(z) = (Q_s + R_s)(1 - \frac{z}{z_i}) + (Q_i + R_i)\frac{z}{z_i} \qquad (2)$$

- Using the same closure assumption proposed by Deardorff (1976),

$$Q_i = -\Delta\theta \frac{dz_i}{dt} = -\frac{A_h}{z_i}\int_0^{z_i} Q(z)dz, \quad \text{with } A_h = 0.5 \qquad (3)$$

- Integrating (2) from 0 to z_i and combining (3), we obtain:

$$\Delta\theta \frac{dz_i}{dt} = \frac{2A_h}{2 + A_h}\left(\frac{Q_s + R_s + R_i}{2} - \frac{1}{z_i}\int_0^{z_i} R(z)dz\right) \qquad (4)$$

- Entrainment rate normalized with convective velocity:

$$E_R = \frac{1}{w_{*R}}\frac{dz_i}{dt} = ARi_R^{-1} \qquad Ri_R \equiv \frac{g}{\theta_0}\frac{\Delta\theta z_i}{w_{*R}^{\ 2}} \qquad w_{*R} \equiv \left[\frac{g}{\theta_0}\left(Q_s + R_s + R_i - \frac{2}{z_i}\int_0^{z_i} R(z)dz\right)z_i\right]^{1/3}$$

Deardorff (1976) closure assumption

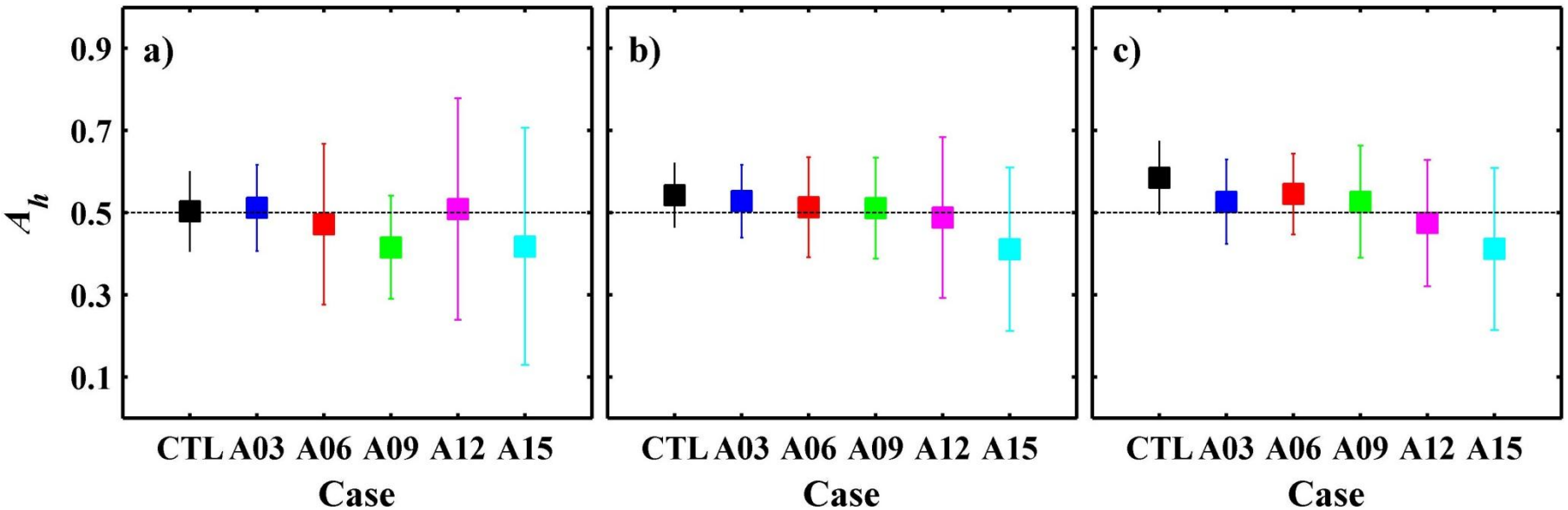


Figure 6. The ratio of A_h in the Deardorff (1976) closure assumption under under a) dθ/dz=3 K km^{-1}, b) dθ/dz=6 K km^{-1}, c) dθ/dz=9 K km^{-1}. Black: CTL, blue: A03, red: A06, green: A09, magenta: A12, cyan: A15.

$$Q_i = -\Delta\theta \frac{dz_i}{dt} = -\frac{A_h}{z_i}\int_0^{z_i} Q(z)dz \quad \text{, where } A_h = 0.5.$$

Evaluation of entrainment equations

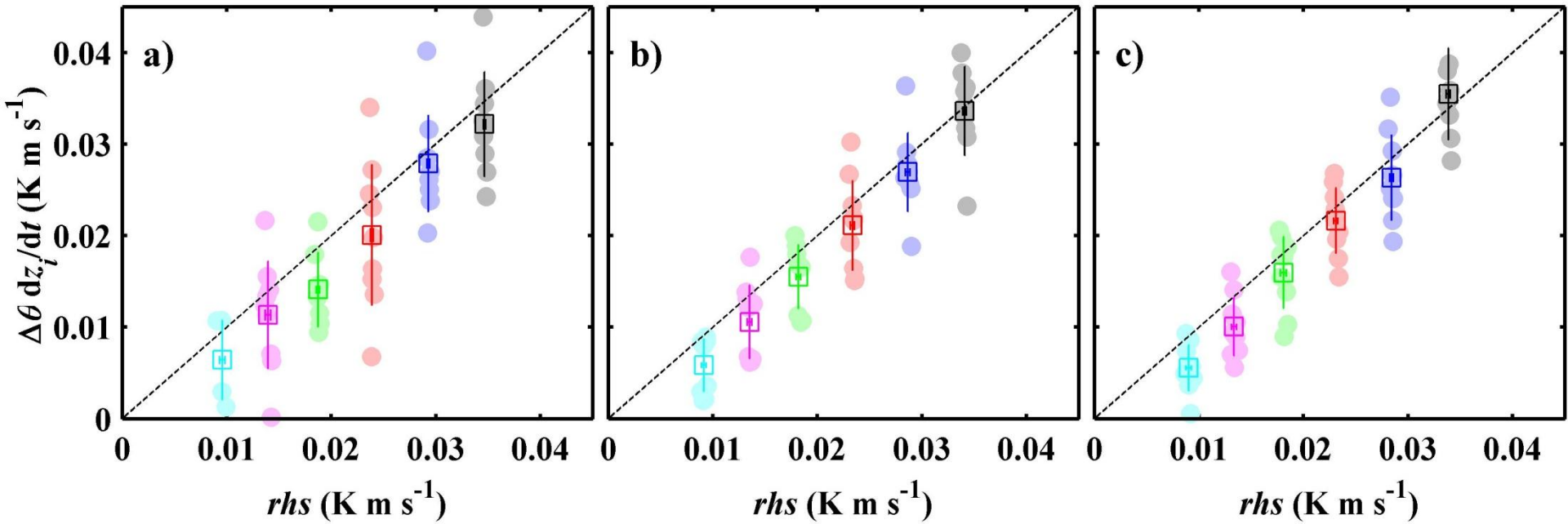


Figure 7. Comparison of right- and left-hand sides of entrainment equation under a) dθ/dz=3 K km^{-1}, b) dθ/dz=6 K km^{-1}, c) dθ/dz=9 K km^{-1}.

$$\Delta\theta \frac{dz_i}{dt} = \frac{2A_h}{2+A_h}\left(\frac{Q_s + R_s + R_i}{2} - \frac{1}{z_i}\int_0^{z_i} R(z)dz\right)$$

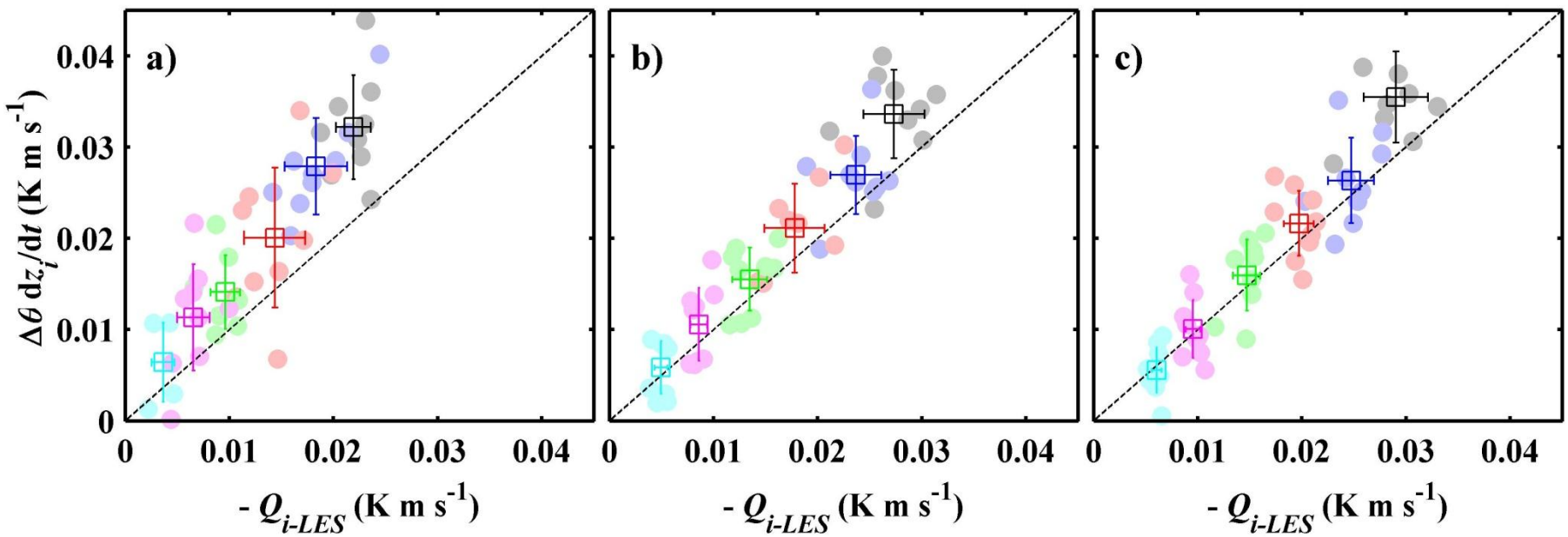


Figure 8. Comparison of left-hand sides of entrainment equation and LES minimum heat flux under a) dθ/dz=3 K km^{-1}, b) dθ/dz=6 K km^{-1}, c) dθ/dz=9 K km^{-1}.

Dimensionless entrainment rate

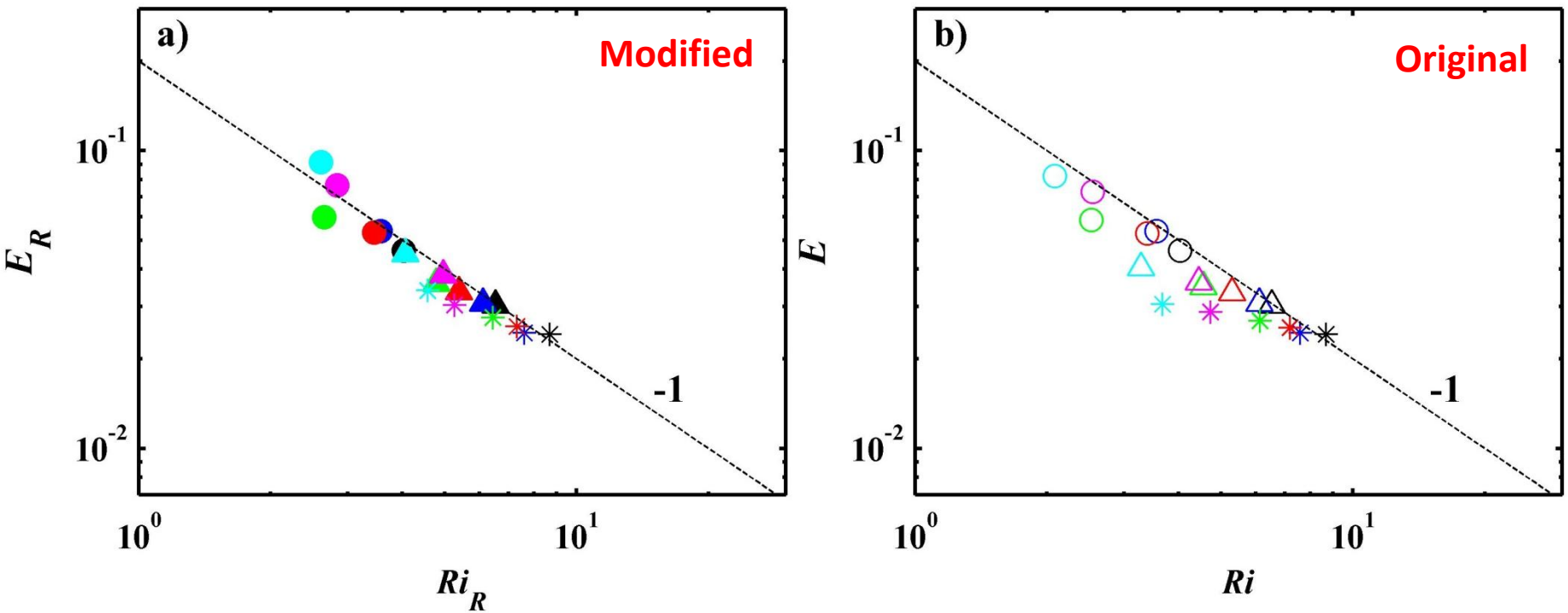


Figure 9. Comparison of original entrainment rate relationship and modified one.

$$E_R = A Ri_R^{-1} \qquad Ri_R \equiv \frac{g}{\theta_0}\frac{\Delta\theta z_i}{w_{*R}^{\ 2}} \qquad w_{*R} \equiv \left[\frac{g}{\theta_0}\left(Q_s + R_s + R_i - \frac{2}{z_i}\int_0^{z_i} R(z)dz\right) z_i\right]^{1/3}$$

Entrainment flux ratio

$$A_i = - Q_i / Q_s$$

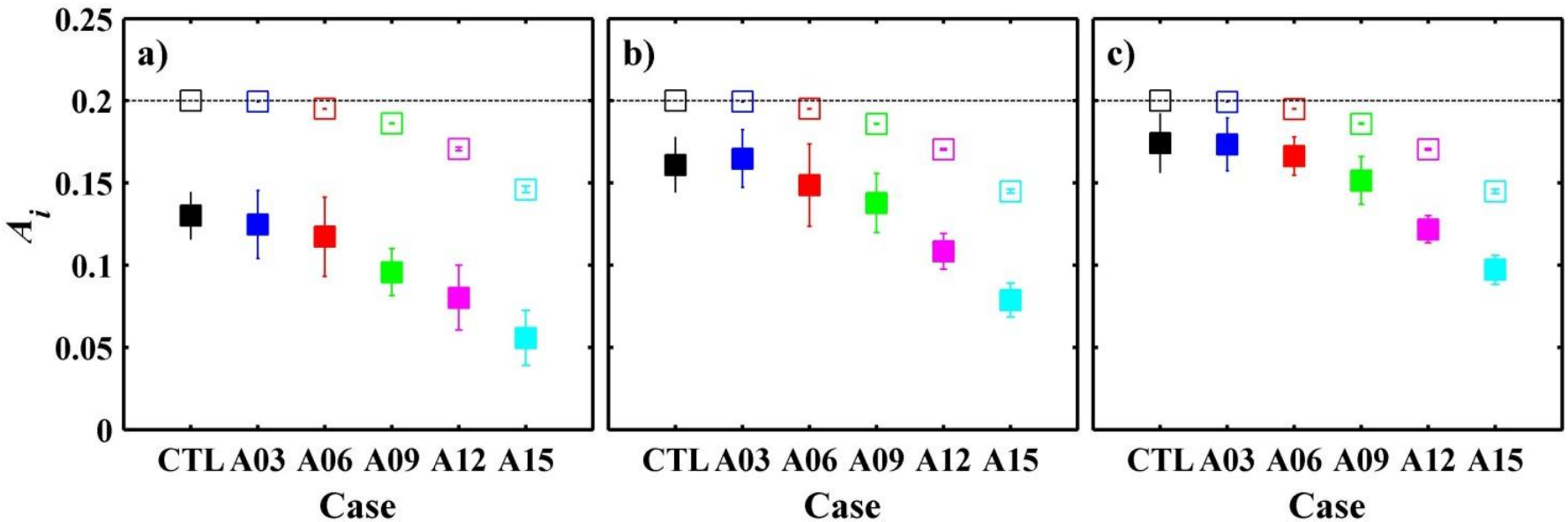
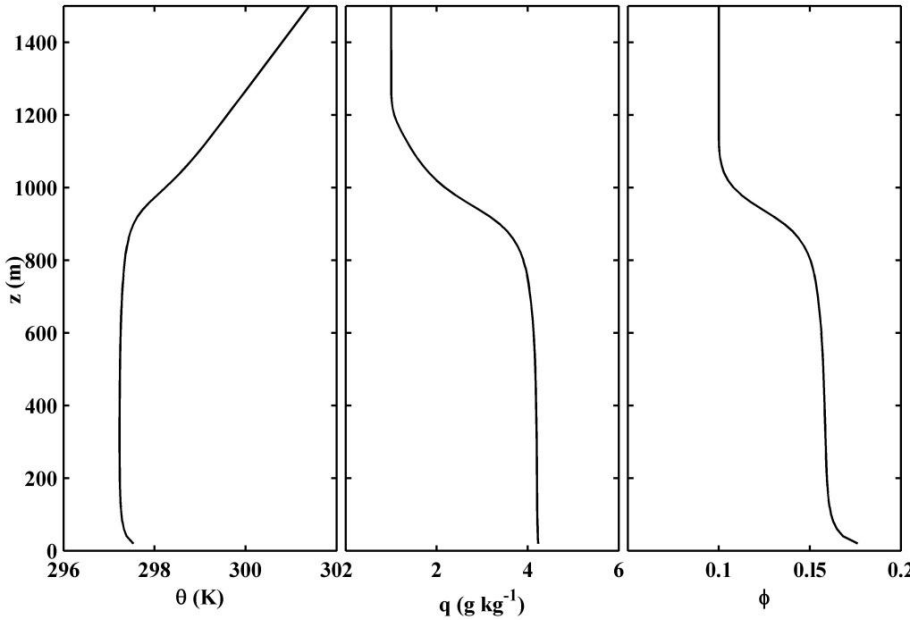


Figure 5. LES and ZOM entrainment ratio for all cases under a) dθ/dz=3 K km^{-1}, b) dθ/dz=6 K km^{-1}, c) dθ/dz=9 K km^{-1}. The error bar represents standard derivation. Box with color filled represent LES ratio, box without color filled is ZOM ratio.

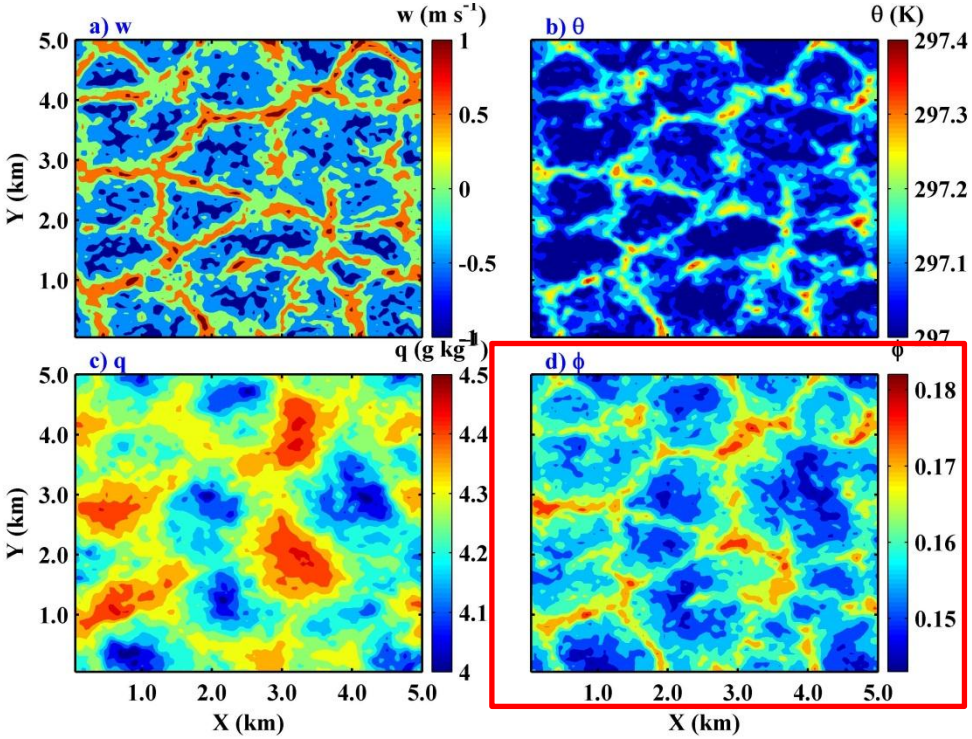
Summary and conclusions

- Aerosol heating changes the temperature and temperature flux profile, the upper boundary layer becomes stable earlier and the profile of temperature flux becomes less linear compared to clean convective boundary layer (CBL).
- When aerosols are presented in boundary layer, both LES and ZOM entrainment flux ratio shows decreasing trend though the surface heat flux reduced by aerosol's absorption and scattering, which is completely opposite to clean CBL, where LES ratio increases with diminishing surface heat flux and ZOM ratio is a constant.
- Derived entrainment rate equation with considering radiative heating term works quite well for all cases. Entrainment rate continues following an inverse relationship with modified Richardson number which includes aerosol radiative heating.

Ongoing work



Adding aerosol tracer to LES.



AOD online calculation

- Assume the component of aerosol is **black carbon**, its density ρ_{BC} is: 2 g cm^{-3}.
- The mass concentration of BC (M_{BC}) in one model layer is: 12 μg m^{-3} (predicted by LES (μg/kg))
- Assume particle is a sphere, its radius is r=1μm, so the volume of one BC particle is: $V_{1,BC}$=4/3 πr^3. then the mass of one particle is: $m_{1,BC}= \rho_{BC} V_{1,BC}$
- The number concentration in this layer is: $n(z)= M_{BC}/ m_{1,BC}$

- The aerosol optical depth: $AOD = \int_0^h n(z)\sigma dz$
- σ is the attenuation cross section, can be calculated by $\sigma=2\pi r^2$. (*Guifu Zhang*, *OU*)
- If aerosol is distributed uniformly within CBL, Then $\boldsymbol{AOD=\sigma n(z_1)\Delta z+ \sigma n(z_2)\Delta z+\ldots+ \sigma n(z_i)\Delta z}$

Thank You !