### **Comments to the Author:**

While the major technical issues have been tackled, there are many English errors or non-standard usages. I just read the title and abstract. A dozen of such problems were noted, as listed below. The paper must be thoroughly edited to drastically improve its English, or it'd be rejected.

### **Response:**

We would like to heartily thank the you for your serious review on our work and the valuable comments. We revised the manuscript in accordance with your kind advices and detailed suggestions, and carefully proof-read the manuscript to minimize typographical, grammatical, and bibliographical errors and improve the English in the manuscript. Here below is our description on revision according to your comments. We sincerely hope the correction will meet with approval.

**Comment 1:** The title is misleading, change to "Evaluating the performance of two surface layer schemes for the momentum and heat exchange processes during severe haze pollution in Jing-Jin-Ji in east China"

### **Response:**

Thanks for pointing this out, and we have changed the title according to the editor's advice.

**Comment 2:** "Pollutants prediction by atmosphere chemical model exists obvious deficiencies," change to "There have existed some deficiencies in the prediction of pollutants by atmosphere chemical models"

## Response:

We have revised the sentence in Lines 21-22, and other similar sentences in Lines 51, 56 have also been revised.

Comment 3: "The differences of two..." should be "The differences between two"

# **Response:**

We changed "of" to "between" in this sentence in Line 24. We also revised similar mistakes in Line 33, Line 170, Line 311, Line 371 and Line 384.

Comment 4: "was mainly evaluated 22 based on". To "was evaluated mainly based on ..."

### Response:

Thank you for your advice. We put "mainly" before "evaluated" to illustrate that we evaluated the performances of the two schemes not only for the pollution process but also for the other times. "mainly" is for "a heavy haze episode", not for "the observed momentum and sensible heat fluxes". So we think it would be more appropriate to put "mainly" before "evaluated". We revised this sentence to make the meaning more clear, and the revision is in Lines 24~26.

Comment 5: "play a major role in the flux calculation" to "play major roles in the flux calculation"

### **Response:**

We changed "play a major role" to "play the major roles" in Line 27. We also corrected other places about singular and plural forms, such as in Line 89, Line 91, Line 272, and Line 335.

Comment 6: "Besides the roughness lengths" to "Besides the roughness length"

# **Response:**

Thanks for pointing this out and we changed "roughness lengths" to "roughness length" as it is a concept here.

**Comment** 7: "the algorithms of universal functions for" either to " the algorithms for" or " the universal functions for" not both algorithms and functions.

## Response:

Thanks for the editor's kind advice. We have deleted "of universal functions" in Line 30.

**Comment 8:** "magnitude of  $z_0 m$  and  $z_0 h$  has" to "the magnitudes of  $z_0 m$  and  $z_0 h$  have"

### **Response:**

We have revised this mistake in Line 31.

## Comment 9: Change all "compared with" to "comparing with"

## **Response:**

We have changed all "compared with" to "comparing with" in the revised manuscript.

Comment 10: "Li scheme better characterized" to "Li scheme is better in characterizing"

# **Response:**

We have revised this mistake in Line 34, and other similar parts were also revised.

Comment 11: "in the describing of" to either " in the description of" or " in describing .."

## **Response:**

Thanks for pointing this mistake out, we have revised all similar problems in whole manuscript.

- 1 Evaluating the performance of two surface layer schemes for the
- 2 momentum and heat exchange processes during severe haze pollution in
- 3 Jing-Jin-Ji in easterneast ChinaEvaluating study of the momentum and
- 4 heat exchange process of two surface layer schemes during severe haze
- 5 pollution in Jing-Jin-Ji in east China

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21 Abstract. The turbulent flux parameterization schemes in the surface layer are crucial for air pollution modeling. -There have 22 existed some deficiencies in the Pollutants prediction of air pollutants by atmosphere chemical models exists obvious 23 deficiencies, which may be closely related to the uncertainties of the momentum and sensible heat fluxes calculated in the 24 surface layer. The differences of between two surface layer schemes (the Li and MM5 schemes) were discussed, and the 25 performances of the two schemes focusing on a heavy haze episode wasere mainly evaluated based on the observed momentum 26 and sensible heat fluxes during a heavy haze episode in Jing-Jin-Ji in eastern China. The results showed that the aerodynamic 27 roughness length  $z_{0m}$  and the thermal roughness length  $z_{0h}$  played thea-major roles in the flux calculation. Compared <u>Comparing</u> with the Li scheme, ignoring the difference between  $z_{0m}$  and  $z_{0h}$  the two i in the MM5 scheme induced a great 28 29 error in the calculation of sensible heat flux (e.g., the error was 54 % at Gucheng station). Besides the roughness lengths, the algorithms of universal functions for surface turbulent fluxes as well as the roughness sublayer also resulted in certain errors 30 31 in the MM5 scheme. In addition, magnitudes of  $z_{0m}$  and  $z_{0h}$  has ve significant influence on the two schemes. The large  $z_{0m}$ 32 and  $z_{0m}/z_{0h}$  in megacity with rough surface (e.g., Beijing) resulted in much larger differences of momentum and sensible 33 heat fluxes by between Li and MM5, compared comparing with the small  $z_{0m}$  and  $z_{0m}/z_{0h}$  in suburban area with smooth 34 surface (e.g., Gucheng). The Li scheme <u>couldis</u> better <u>in-</u>characterizeinged the evolution of atmospheric stratification than the

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Tong Jiang<sup>5</sup>, Huizheng Che<sup>1</sup>, Meng Zhang<sup>6</sup></sup> 

- MM5 scheme in general, especially for the transition stage from unstable to stable atmospheric stratification corresponding to the PM<sub>2.5</sub> accumulation. The biases of momentum and sensible heat fluxes from Li were lower about 38 % and 43 % respectively than those from MM5 during this stage. This study indicates the superiority of the Li scheme in the describing of the regional atmospheric stratification, and also suggests the with improving possibility of severe haze prediction in Jing-Jin-Ji in eastern China by coupling it into-the atmosphere chemical models-online.
- 40 Key words: surface layer; turbulent flux parameterization; roughness length; numerical modeling; air pollution

### 41 1 Introduction

42 Adequate air quality modeling relies on accurate simulation of meteorological conditions, especially in the planetary 43 boundary layer (PBL) (Hu et al., 2010; Cheng et al., 2012; Xie et al., 2012). The PBL is tightly coupled towith the earth's 44 surface by turbulent exchange processes. As the bottom layer of PBL, the surface layer (SL) reflects the surface state by 45 calculating momentum, heat, water vapor and other fluxes, and influences the atmospheric structure by turbulent transport 46 process. Many studies have illustrated the important roles of meteorological factors in the SL during in the formation of air 47 pollution formation. It has been They demonstrated that weak wind speed, high relative humidity (RH) and strong temperature 48 inversion are favorable for the haze concentrating (Zhang et al., 2014; Yang et al., 2015; Liu et al., 2017; Zhong et al., 2017). 49 The strong stable stratification and weak turbulent are mainly responsible for many haze events. The relationship between flux 50 and atmospheric profile in the atmospheric surface layer is a critical factor for air pollution diffusion, especially under stable 51 stratification conditions (Li et al., 2017). However, there are the study of stable boundary layer-still has-some uncertainties in 52 the study of stable boundary layer due to the poor description of surface turbulent motion. The simulating study on a severe 53 haze in eastern China by the Weather Research and Forecasting/Chemistry (WRF-Chem) model concluded that there is lower 54 ability of current PBL schemes hads a weak ability toin distinguishing the diffusion between haze days under stable conditions 55 and clean days under unstable conditions (Li et al., 2016a). Another study (Vautard et al. 2012) onof mesoscale meteorological 56 models also pointed out there was a systematic overestimation of near-surface wind speed in thea stable boundary layer which 57 and its possible should contributeion to the underestimation of the PM2.5 pollution.s urface concentrations of primary pollutions. 58 In addition, atmospheric conditions in both the PBL and upper layers are highly dependent on the turbulent fluxes which are 59 computed in the SL (Ban et al., 2010). Flux parameterization in the SL plays an important role in studies of the hydrological 60 cycle and weather prediction (Yang et al., 2001; Li, 2014). An adequate SL scheme is crucial to provide an accurate atmospheric evolution by numerical models (Jiménez et al., 2012) and hence it may introduce significant impacts on air 61 62 pollution simulation.

63 The bulk aerodynamic formulation based on Monin-Obukhov similarity theory (hereinafter MOST, Monin and Obukhov,
 64 1954) is usually employed to calculate surface fluxes in numerical models. Turbulent fluxes are parameterized by wind,

65 temperature, humidity in the lowest layer in the model and temperature and humidity at the surface. Many international scholars 66 verified the MOST using field experiments and then proposed the universal functions, the commonly used of which is 67 Businger-Dyer (BD) equation (Businger, 1966; Dyer, 1967). With the development of observation technology, the coefficients in the BD equation have been further modified (Paulson, 1970; Webb, 1970; Businger et al., 1971; Dyer, 1974; Högström, 68 69 1996). In addition to the BD equation, some other schemes have been put forward and they performed better especially for 70 strongly stable stratification (Holtslag and De Bruin, 1988; Beljaars and Holtslag, 1991; Cheng and Brutsaert, 2005). The 71 schemes can be divided into two types according to the computing characteristics. One type is called as iterative algorithm 72 (Paulson, 1970; Businger et al., 1971; Dyer, 1974; Högström, 1996; Beljaars and Holtslag, 1991), and it keeps the MOST 73 completely with less approximation so that the results can be more precise. However, it needs to take much more steps to 74 converge and hence the CPU time is consuming which reduces the computational efficiency of modeling (Louis, 1979; Li et 75 al., 2014); The other one is called as non-iterative algorithm (Louis et al., 1982; Launiainen, 1995; Wang et al., 2002; Wouters 76 et al., 2012). There is no requirement for loop iteration in the calculation due to the approximate treatment. This algorithm is 77 much simpler and less CPU time-consuming, but the results are based on the loss of the calculation accuracy.

78 A new non-iterative scheme proposed by Li et al. (2014; 2015, Li hereinafter) speeds up effectively under a higher 79 accuracy compared comparing with some classic iterative computation. It is remarkable that this new scheme just has been 80 theoretically evaluated and it has never been applied in any models. Haze pollution occurs frequently in recent years in eastern China. The concentration of PM<sub>2.5</sub> may reach up to 1000  $\mu$ g m<sup>-3</sup> in the Beijing-Tianjin-Hebei (Jing-Jin-Ji) region in winter 81 82 (Wang et al., 2014) while it is was generally underestimated by current air quality models (Zhang et al., 2015; Li et al., 2016a; 83 Liu et al., 2017). The Li and another classic SL scheme (Zhang and Anthes, 1982, MM5 hereinafter) are-were compared in 84 details in this study. The observed momentum and sensible heat flux data covering one complete haze process at Gucheng 85 station were used to evaluate the two schemes focusing on the transition stage from unstable to stable atmospheric stratification 86 corresponding to the PM<sub>2.5</sub> accumulation. The evaluation is in the view of both local and regional scales. This offline-study 87 may provide the prerequisite for the online-coupling the Li scheme into atmosphere chemical models in the future.

### 88 2 Theory

93

89 The definitions of momentum and sensible heat flux as well as the detailed algorithms of the Li and MM5 schemes are
90 introduced in this section.

## 91 2.1 Introduction of the momentum and sensible heat flux

92 The turbulent fluxes from ground surface are defined as follows:

$$\tau = \rho u_*^2,\tag{1a}$$

94 
$$H = -\rho c_n u_* \theta_*, \tag{1b}$$

- 95 where  $\tau$  is the momentum flux, H is the sensible heat flux,  $\rho$  is the air density,  $c_p$  is the specific heat capacity at constant 96 pressure.  $u_*$  and  $\theta_*$  are the friction velocity and the temperature scale, respectively, and they represent the intensity of the 97 vertical turbulent flux transport and are approximately independent on height in the SL.
- 98 Both the Li and MM5 schemes are calculated withbased on bulk flux parameterization. As an important dimensionless 99 parameter related to the stability, the bulk Richardson number  $Ri_B$  is defined as
- $Ri_{\rm B} = \frac{gz(\theta \theta_{\rm g})}{\theta u^2},$ 100 (2)

101 where g is the acceleration of gravity, z is the reference height which is the lowest level in the models,  $\theta$  is the mean potential 102 temperature at height z,  $\theta_{g}$  is the surface radiometric potential temperature, u is the mean wind speed at height z. Thus,  $Ri_{B}$ 103 can be computed through meteorological variables from at least two levels.

#### 104 2.2 The Li scheme

105 This new scheme employs non-iterative algorithm to compute the surface fluxes. Its basic idea is to parameterize the 106 stability parameter  $\zeta$  directly with  $Ri_B$  and roughness lengths ( $z_{0m}$  and  $z_{0h}$ ). Specifically, bulk transfer coefficients of the 107 momentum and sensible heat fluxes ( $C_M$  and  $C_H$ ) are expressed as

108 
$$C_M = \frac{u_*^2}{u^2} = \frac{\tau}{\rho u^2},$$
 (3a)

109 
$$C_H = \frac{u_*\theta_*}{u(\theta - \theta_g)} = -\frac{H}{\rho c_p u(\theta - \theta_g)}.$$
 (3b)

110 Based on MOST and considering the roughness sublayer (RSL) effect at the same time, the relationships between the 111 bulk transfer coefficients and the profile functions corresponding to wind and potential temperature are usually expressed as

112 
$$C_{M} = \frac{k^{2}}{\left[\ln \frac{z}{z_{0m}} - \psi_{M}\left(\frac{z}{L}\right) + \psi_{M}\left(\frac{z}{L}, \frac{z}{z_{*}}\right)\right]^{2}},$$
 (4a)

113 
$$C_{H} = \frac{k^{2}}{R\left[\ln\frac{z}{z_{0m}} - \psi_{M}\left(\frac{z}{L}\right) + \psi_{M}\left(\frac{z_{0m}}{L}\right) + \psi_{M}^{*}\left(\frac{z}{L}, \frac{z}{z_{s}}\right)\right]\left[\ln\frac{z}{z_{0h}} - \psi_{H}\left(\frac{z}{L}\right) + \psi_{H}\left(\frac{z}{L}, \frac{z}{z_{s}}\right)\right]}, \tag{4b}$$

114 where k is the von Kármán constant which is 0.4 in both two schemes, R is the Prandtl number which is 1.0 in the two 115 schemes,  $z_{0m}$  and  $z_{0h}$  are the aerodynamic roughness length and the thermal roughness length, respectively.  $\psi_M$  and  $\psi_H$ 116 are the integrated stability functions for momentum and sensible heat, respectively, which are also called universal functions. L is the Obukhov length  $(\zeta = \frac{z}{L})$ ,  $\psi_M^*$  and  $\psi_H^*$  are the correction functions accounting for RSL effect,  $z_*$  is the RSL height. 117 118 It is clear to see that the calculation of the momentum and sensible heat fluxes requires  $C_M$  and  $C_H$  (or  $u_*$  and  $\theta_*$ ), and 119 there are 3 key points to get them:

120 1.  $z_{0m}$  and  $z_{0h}$ .  $z_{0m}$  and  $z_{0h}$  are two key parameters in the bulk transfer equations. Their definitions and influences 121 will be discussed in Sect. 4.1. Note that both  $z_{0m}$  and  $z_{0h}$  are taken into account by the Li scheme. In other words, the 122 Li scheme distinguishes these two principal surface parameters effectively as they generate from different mechanisms. 123

2.  $\zeta$ . The determination of  $\zeta$  is the most crucial problem forin the Li scheme. In fact, this new scheme consists of two

parts. The first part wasis proposed for atmospheric stable stratification conditions (Li et al., 2014), and the second part then extendsed the scheme to unstable conditions (Li et al., 2015). For stable conditions, the calculation procedure for a given group of  $Ri_B$ ,  $z_{0m}$  and  $z_{0h}$  is the following: (1) find the region according to  $z_{0m}$  and  $z_{0h}$ ; (2) find the section according to the region and  $Ri_B$  with Eq. (5) and given coefficients; (3) calculate  $\zeta$  using Eq. (6) and given coefficients.

128 
$$Ri_{Bcp} = \sum C_{mn} (\log L_{0M})^m (L_{0H} - L_{0M})^n,$$
(5)

$$\zeta = Ri_{\rm B} \sum C_{ijk} Ri_{\rm B}^i L_{0M}^j (L_{0H} - L_{0M})^k, \qquad (6)$$

where  $C_{mn}$  and  $C_{ijk}$  are the coefficients <u>listed</u> in Tables in Li et al. (2014).  $L_{0M} = \ln \frac{z}{z_{0m}}$ ,  $L_{0H} = \ln \frac{z}{z_{0h}}$ . m, n = 0, 1, 2, ...

and  $m + n \le 3$ ; i, j, k = 0, 1, 2, 3, and i + j + k  $\le 4$ . Similarly, for unstable conditions, eight regions are divided according to the method from Li et al. (2015). For each of the regions,  $\zeta$  is carried out by following:

133 
$$\zeta = Ri_{\rm B} \frac{L_{0M}^2}{L_{0H}} \sum C_{ijk} \left( \frac{-Ri_{\rm B}}{L_{0H}} \right)^i L_{0M}^{-j} L_{0H}^{-k}, \tag{7}$$

134 where  $C_{ijk}$  is listed in Li et al. (2016b), and i = 0, 1; j, k = 0, 1, 2, 3;  $i + j + k \le 4$ .

3. Universal function. It is also a key factor in flux calculation. The form of universal function here is adopted from Cheng
and Brutsaert (2005) under the stable conditions (Eqs. (8a), (8b)) and it is adopted from Paulson (1970) under the unstable
conditions (Eqs. (9a), (9b)):

$$\psi_M(\zeta) = -a \ln\left[\zeta + (1+\zeta^b)^{\frac{1}{b}}\right], \quad \zeta > 0 \quad (\text{stable}), \tag{8a}$$

139 
$$\psi_H(\zeta) = -c \ln \left[\zeta + (1+\zeta^d)^{\frac{1}{d}}\right], \quad \zeta > 0 \text{ (stable)}, \tag{8b}$$

140 
$$\psi_M(\zeta) = 2\ln\frac{1+x}{2} + \ln\frac{1+x^2}{2} - 2\arctan(x) + \frac{\pi}{2}, \quad \zeta < 0 \text{ (unstable)}, \tag{9a}$$

141

138

129

$$\psi_H(\zeta) = 2\ln\frac{1+y}{2}, \quad \zeta < 0 \quad \text{(unstable)},$$
 (9b)

142 where  $a = 6.1_{a}$ ,  $b = 2.5_{a}$ ,  $c = 5.3_{a}$ ,  $d = 1.1_{a}$ ,  $x = (1 - 16\zeta)^{1/4}$ ,  $y = (1 - 16\zeta)^{1/2}$ .

In addition, the RSL effect is taken into account in the Li scheme. The definitions and influence of RSL will also be discussed in Sect. 4.1. De Ridder (2010) proposed the expression of  $\psi_M^*$  and  $\psi_H^*$ :

145 
$$\psi_M^*\left(\zeta, -\frac{z}{z_*}\right) = \phi_M\left[\left(1 + \frac{v}{\mu_M z/z_*}\right)\zeta\right]\frac{1}{\lambda}\ln\left(1 + \frac{\lambda}{\mu_M z/z_*}\right)e^{-\mu_M z/z_*},\tag{10a}$$

$$\psi_H^*\left(\zeta, - \frac{z}{z_*}\right) = \phi_H\left[\left(1 + \frac{v}{\mu_H z/z_*}\right)\zeta\right]\frac{1}{\lambda}\ln\left(1 + \frac{\lambda}{\mu_H z/z_*}\right)e^{-\mu_H z/z_*},\tag{10b}$$

147 where  $v = 0.5_{a^{-}} \mu_{M} = 2.59_{a^{-}} \mu_{H} = 0.95$ ,  $z_{*} = 16.7 z_{0m^{a^{-}}} \lambda = 1.5$ .  $\phi_{M}$  and  $\phi_{H}$  are universal functions before 148 integration. Here, set  $\chi_{M} = 1 + \frac{v}{\mu_{M} z/z_{*}} \chi_{H} = 1 + \frac{v}{\mu_{H} z/z_{*}}$ :

149  
$$\phi_{M}(\chi_{M}\zeta) = 1 + a \frac{\chi_{M}\zeta + (\chi_{M}\zeta)^{b} [1 + (\chi_{M}\zeta)^{b}]^{\frac{1-b}{b}}}{\chi_{M}\zeta + [1 + (\chi_{M}\zeta)^{b}]^{\frac{1}{b}}}, \quad \zeta > 0 \text{ (stable)}, \quad (11a)$$

150 
$$\phi_H(\chi_H\zeta) = 1 + c \frac{\chi_H\zeta + (\chi_H\zeta)^d [1 + (\chi_H\zeta)^d]^{\frac{1-a}{d}}}{\chi_H\zeta + [1 + (\chi_H\zeta)^d]^{\frac{1}{d}}}, \quad \zeta > 0 \text{ (stable)}, \quad (11b)$$

151 
$$\phi_M(\chi_M \zeta) = (1 - 16\chi_M \zeta)^{-1/4}, \quad \zeta < 0 \text{ (unstable)},$$
 (12a)

152 
$$\phi_H(\chi_H\zeta) = (1 - 16\chi_H\zeta)^{-1/2}, \quad \zeta < 0 \text{ (unstable)}.$$
 (12b)

#### 153 2.3 The MM5 scheme

154 The MM5 scheme is a classic one which is widely applied in modeling investigation (Hu et al., 2010; Wang et al., 2015a, 155 b; Tymvios et al., 2017). This scheme does not distinguish  $z_{0h}$  from  $z_{0m}$ , thus the roughness length here is expressed as  $z_0$ . 156 For unstable conditions, the function forms are given by Eqs. (16a) and (16b) following Paulson (1970), and for stable 157 conditions, the atmospheric stratification conditions are subdivided into three cases according to Zhang and Anthes (1982) and 158 the function forms are given by Eqs. (13), (14), and (15).

159 (1) Strongly stable condition ( $Ri_B \ge 0.2$ ):

160 
$$\psi_M = \psi_H = -10 \ln \frac{z}{z_0}$$
. (13)

161 (2) Weakly stable condition ( $0 < Ri_B < 0.2$ ):

162 
$$\psi_M = \psi_H = -5 \left(\frac{Ri_B}{1.1 - 5Ri_B}\right) \ln \frac{z}{z_0}.$$
 (14)

- 163 (3) Neutral condition ( $Ri_{\rm B} = 0$ ):
- $\psi_M=\psi_H=0.$ 164
- 165 (4) Unstable condition ( $Ri_{\rm B} < 0$ ):
- $\psi_M = 2 \ln \frac{1+x}{2} + \ln \frac{1+x^2}{2} 2 \arctan(x) + \frac{\pi}{2},$ (16a)

166

 $\psi_H = 2\ln\frac{1+y}{2},$ (16b)

(15)

168 where  $x = (1 - 16\zeta)^{1/4} - y = (1 - 16\zeta)^{1/2}$ .

169 This scheme calculates turbulent fluxes of the momentum and sensible heat with  $u_*$  and  $\theta_*$ . In order to avoid the huge 170 difference of  $u_{\pm}$  through between the two computations,  $u_{\pm}$  is arithmetically averaged with its previous value by Eq. (17), 171 and a lower limit of  $u_* = 0.1 \text{ m/s}$  is imposed to prevent the heat flux from being zero under very stable conditions. According 172 to the profile functions of wind and temperature near the ground,  $\theta_*$  then is then deduced by Eq. (18).

173  
174  

$$u_{*} = \frac{1}{2} \left( u_{*} + \frac{ku}{\ln \frac{z}{z_{0m}} - \psi_{M}} \right), \quad (17)$$

$$\theta_{*} = \frac{k(\theta - \theta_{g})}{R [\ln \frac{z}{z_{0h}} - \psi_{H}]}. \quad (18)$$

174

175 The calculation procedure of the Li scheme is the following: (1) determine  $Ri_{B} - z_{0m}$  and  $z_{0h}$  according to the 176 observation data; (2) calculate  $\zeta$  with  $Ri_{B_{a}} - z_{0m}$  and  $z_{0h}$ ; (3) calculate the momentum and sensible heat fluxes under 177 different conditions. The MM5 scheme is summarized as follows: (1) determine the universal functions according to the values

of  $Ri_{\rm B}$  and  $z_0$ ; (2) calculate the  $u_*$  and  $\theta_*$  with the meteorological variables and flux data; (3) derive the turbulent fluxes. **Compared**-<u>Comparing</u> with other non-iterative schemes including MM5, the Li scheme can be applied to the full range of roughness status  $10 \le \frac{z}{z_{0m}} \le 10^5$  and  $-0.5 \le \ln \frac{z_{0m}}{z_{0h}} \le 30$  under whole conditions\_ $-5 \le Ri_{\rm B} \le 2.5$ . In addition, there are three obvious differences between the Li and MM5 schemes: (1) Li distinguishes  $z_{0h}$  from  $z_{0m}$  but MM5 does not distinguish them; (2) the two schemes apply different universal functions under stable conditions; (3) Li considers the RSL effect while MM5 ignores it.

## 184 3 Observational data and methods

185 The observational fluxes used in this study were measured at Gucheng station from December 1, 2016 to January 9, 2017. 186 Gucheng station (115.40 ° E, 39.08 ° N) is located at Gucheng County, Baoding, Hebei province and it is about 110km 187 southwest of Beijing (Fig. 1a). This station has a farmland site where rice is planted grown in summer and wheat in winter. 188 The surroundings are mainly farmland and scattered villages (Fig. 1b). At Gucheng station, the momentum and sensible heat 189 fluxes near the surface were measured by the eddy correlation flux measurement system. The system is mainly composed of a 190 sonic anemometer (CSAT3) and a gas analyzer (LI-7500). They are set up at 4 m height above the surface ground. The 191 measured fluxes are used to evaluate the two schemes as well as estimate the roughness lengths. The measured meteorological 192 variables including wind speed and direction, temperature, humidity, pressure, radiation are utilized to calculate the momentum 193 and sensible heat fluxes both in the Li and MM5 schemes. Note the observed meteorological data were from Gucheng station 194 and national basic automatic weather stations in Jing-Jin-Ji in eastern China, respectively. Hourly surface PM2.5 mass 195 concentration in Baoding and Beijing from China National Environmental Monitoring Centre (http://www.cnemc.cn/) was 196 also used in this paper.

### 197 3.1 Data processing

To obtain accurate flux data, quality control has been performed for the observational data, including: (1) eliminate the outliers and the data in rainy days; (2) double rotation and WPL correction (Webb et al., 1980); (3) omit the dataset when the wind speed is less than 0.5 m s<sup>-1</sup>. In addition, the wind field especially the wind direction has a great impact on the value of  $z_{0m}$ , so it is necessary to understand the situation at Gucheng station. Figure 2 shows the distribution frequency of wind speed and wind direction at Gucheng during the observation (December 1, 2016 ~ January 9, 2017). The wind speed is stable during this period and the maximum is no more than 5 m s<sup>-1</sup> and most of them are about 1 ~ 2 m s<sup>-1</sup>. The wind direction is relatively uniform except for the southeast wind (135 °).

## 205 **3.2 Determination of surface skin temperature**

206 The surface skin temperature at Gucheng station is calculated from the radiation data by the following formula:

207 
$$R_{lw}^{\uparrow} = (1 - \varepsilon_s) R_{lw}^{\downarrow} + \varepsilon_s \sigma T_g^4, \qquad (19)$$

208 where  $R_{lw}^{\uparrow}$  and  $R_{lw}^{\downarrow}$  are the surface upward longwave radiation and long wave radiation incident on the surface, respectively.  $\sigma$  is the Stephen Boltzmann constant,  $\sigma = 5.67 \times 10^{-8}$  W m<sup>-2</sup> K<sup>-4</sup>.  $T_g$  is the surface skin temperature,  $\varepsilon_s$  is 209 210 the surface emissivity which is the prerequisite <u>offer calculating</u>  $T_g$  <u>calculation</u>. Many researches estimated the value of  $\varepsilon_s$ 211 and found the range of the values <u>it</u> is always  $0.9 \sim 1$  (Stewart et al., 1994; Verhoef et al., 1997). According to the semi-212 empirical method in Yang et al. (2008),  $\varepsilon_s$  is estimated when the RMSE is minimal. In this paper, the Li and MM5 schemes 213 were used to estimate the  $\varepsilon_s$  value (as shown in Fig. 3). It is clear that the  $\varepsilon_s$  value corresponding to the minimum RMSE is 214 not very sensitive to the choice of two schemes. When  $\varepsilon_s$  is 1, the RMSE has the minimum value. Thus, this experiment takes 215 1 as the optimal value of  $\varepsilon_s$ .

# 216 3.3 Determination of roughness length $z_{0m}$ ( $z_{0h}$ )

Using the observed momentum and sensible heat fluxes and the meteorological variables including wind speed, temperature, humidity and pressure after quality control at Gucheng station,  $z_{0m}$  and  $z_{0h}$  were derived from Eqs. (20a) and (20b) following Yang et al. (2003) and Sicart et al. (2014).

$$\frac{u_*}{u} = \frac{k}{\ln\frac{z}{z_{0m}} - \psi_M},\tag{20a}$$

221 
$$\frac{\theta_*}{(\theta - \theta_g)} = \frac{k}{R[\ln \frac{z}{z_{0h}} - \psi_H]}.$$
 (20b)

During the observation period, the crops stopped growing and the height did not exceed 0.1 m, so the zero-plane displacement height was ignored henceand the reference height z was taken as 4m. The observation time was too short (about 1 month) to consider the effect of seasonal variations on the roughness lengths. Thus,  $z_{0m}$  and  $z_{0h}$  were assumed as two fixed values. Based on the variables and formulae mentioned above, the two roughness lengths at Gucheng are derived:  $z_{0m} =$ 0.0419 m,  $z_{0h} = 0.0042$  m.

# 227 4 Results and discussion

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The <u>definitions and influences of RSL</u>, roughness length and their influence on the calculation of turbulent flux are discussed in detail in this section. The Li and MM5 schemes are <u>offline</u> tested <u>offline</u> and evaluated during the haze pollution from December 13 to 23, 2016.

# 4.1 The influence<u>s</u> of RSL and roughness length on the calculation of turbulent flux

The RSL is usually defined as the region where the flow is influenced by the individual roughness elements as reflected by the spatial inhomogeneity of the mean flow (Florens et al., 2013). In the RSL, turbulence is strongly affected by individual roughness elements, and the standard MOST is no longer valid (Simpson et al., 1998). Therefore, it is necessary to consider 235 the RSL effect in the calculation of turbulent flux, especially for the rough terrain such as forest or large cities.  $z_{0m}$  is defined 236 as the height at which the extrapolated wind speed following the similarity theory vanishes. It is mainly determined by land-237 cover type and canopy height after excluding large obstructions. In models,  $z_{0m}$  is always based on the look-up table which 238 is related to land-cover types. In this study,  $z_{0m}$  was simply classified based on the research of Stull (1988) and listed in 239 Table 1. It can be seen in Table 1 that the rougher underlying surface corresponds to the larger value of  $z_{0m}$ .  $z_{0h}$  is the height 240 at which the extrapolated air temperature is identical to the surface skin temperature. Some early researchers assumed that 241  $z_{0m}$  was equal to  $z_{0h}$  (Louis, 1979; Louis et al., 1982). However, the assumption is not applicable in reality because  $z_{0m}$ 242 and  $z_{0h}$  have different physical meanings. Different treatments of  $z_{0m}$  and  $z_{0h}$  may introduce considerable changes in the 243 surface flux calculation (Launiainen, 1995; Kot and Song, 1998; Anurose and Subrahamanyam, 2013). Many studies removed 244 the assumption that  $z_{0m}$  was equal to  $z_{0h}$  and made the schemes more applicable in the situation that  $z_{0m}$  was not equal to  $z_{0h}$  or the ratio of  $z_{0m}$  to  $z_{0h}$  was much large (Wouters et al., 2012; Li et al., 2014; Li et al., 2015). Some field experiments 245 246 even indicated the ratio  $z_{0m}/z_{0h}$  has a diurnal variation (Sun, 1999; Yang, 2003; Yang, 2008). In this study, we make the 247 common assumption that the ratio  $z_{0m}/z_{0h}$  is a constant.

248 Considering the lowest level in mesoscale models is usually about 10m, z = 10 m is set as the reference height in this 249 study. The range of  $Ri_B$  is set according to Louis 82 (Louis et al., 1982) in the following discussion. Firstly, the study discusses 250 the effects of different land-cover types (different  $z_{0m}$  values) and RSL on flux calculation-were discussed. Set  $z_{0m} = z_{0h}$ , 251 corresponding to four cases:  $z_{0m} = 1, 0.5, 0.05, 0.001$  m. These cases correspond to large cities, forests, agricultural fields and 252 wide water surface, respectively. Figure 4 shows the relationship between  $C_M(C_H)$  and  $Ri_B$  for <u>inunder</u> different  $z_{0m}$  values 253 and treatments of RSL. It can be seen that both RSL and  $z_{0m}$  have impacts on  $C_M$  and  $C_H$ . Ignoring the RSL effect can results in lager  $C_M$  and  $C_H$ , compared comparing with the results of original scheme considering the RSL effect. The 254 255 difference induced by RSL <u>effect</u> is evident only under the rough surface. For example, the difference under  $z_{0m} = 1$  is 256 obviously greater than other  $z_{0m}$  settings, and when  $z_{0m}$  is reduced to 0.05 or less, the RSL has little effect. Furthermore, 257 the RSL contributes more to sensible heat transfer than to momentum transfer under the same setting of  $z_{0m}$ . The effects of 258 different land-cover types on  $C_M$  and  $C_H$  are much more significant compared comparing with RSL. The rougher the surface 259 is (corresponding to the larger  $z_{0m}$  value) brings, -the larger the  $C_M$  ( $C_H$ ) is under the same stability. In addition, there is a 260 corresponding relationship between  $C_M(C_H)$  and stability. The more unstable the atmosphere is, the larger difference t<u>T</u>he 261 value of  $C_M(C_H)$  drops is and vice versa with the stability. Once  $Ri_B$  exceeds the critical value (generally 0.2 ~ 0.25), the 262 transfer coefficients decline sharply but still above 0.

Secondly, the effects of difference between  $z_{0m}$  and  $z_{0h}$  as well as RSL on flux calculation are discussed. The relationship between  $z_{0m}$  and  $z_{0h}$  can be expressed as  $kB^{-1} = \ln \frac{z_{0m}}{z_{0h}}$ . Over the sea,  $z_{0m}$  is comparable to  $z_{0h}$ ; over the uniform vegetation surface (e.g., grassland, farmland, woodland),  $kB^{-1}$  is about 2 ( $z_{0m}/z_{0h} \approx 10$ ) (Garratt and Hicks, 1973; 266 Garratt, 1978; Garratt and Francey, 1978), which coincides with our results in Gucheng ( $z_{0m} = 0.0419 \text{ m}$ ,  $z_{0h} = 0.0042 \text{ m}$ ); 267 over the surface with bluff roughness elements, the  $kB^{-1}$  value may be very large. For example, in some large cities,  $kB^{-1}$ 268 is even up to 30  $(z_{0m}/z_{0h} \approx 10^{13})$  (Sugawara and Narita, 2009). Therefore, the ratio  $z_{0m}/z_{0h}$  varies over a wide range. 269 Figure 5 shows the relationship between  $C_M(C_H)$  and  $Ri_B$  <u>underfor different treatments</u> of  $z_{0m}/z_{0h}$ . Set  $z_{0m} = 1$  as a large 270 city case,  $z_{0h}=1$ , 0.01, 10<sup>-4</sup>, 10<sup>-6</sup> m, and the large differences derived from the different ratios are displayed in Fig. 5. The 271 similar RSL effect can be found compared with Fig. 4. The differences induced by RSL effect are more obvious than that ose 272 in Fig. 4. The different treatments of ratio  $z_{0m}/z_{0h}$  haves great impacts on turbulent flux transfer, particularly for sensible 273 heat transfer. It seems evident that when  $z_{0h}$  is not equal to  $z_{0m}$  ( $z_{0m}/z_{0h}=100 \sim 10^6$ ), the calculated  $C_H$  is much small 274 compared to the treatment that  $z_{0h}$  is equal to  $z_{0m}$  ( $z_{0m}/z_{0h}=1$ ). In addition,  $C_M(C_H)$  decreases with the increase of 275 stability, and <u>itthey</u> decreases much slower when  $z_{0h}$  is not equal to  $z_{0m}$ .

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# 277 4.2 Comparison of momentum and sensible heat fluxes calculated by the two schemes

278 Using the obtained roughness lengths and the observations, the momentum and sensible heat flux were calculated by the 279 Li and MM5 schemes. Firstly,  $z_{0m}$  and  $z_{0h}$  were set as 0.0419 and 0.0042 respectively in the Li scheme,  $z_0$  was equal to 280  $z_{0m}$  in the MM5 scheme to calculate the momentum and sensible heat fluxes and the results are shown in Figs. 6a and 6b. It 281 can be seen that compared comparing with MM5, Li performs better with higher regression coefficient and determination 282 coefficient. For the momentum fluxes, the regression coefficient by Li is 0.6795 and that by MM5 is 0.5598, indicating that 283 the error of Li is 12 % lower than that of MM5. For sensible heat fluxes, the regression coefficient by Li is 0.7967 and that by 284 MM5 is 1.7994. The latter is much larger than 1, that is, the MM5 scheme obviously overestimates the sensible heat due to it 285 does not distinguish  $z_{0h}$  from  $z_{0m}$ . Then, make  $z_0$  equal to 0.0042 in the MM5 scheme to re-calculate the sensible heat 286 fluxes and the result is as shown in Fig. 6c. It can be seen the result has a great improvement after modifying  $z_0$  value and the 287 regression coefficient by MM5 is 0.7363, indicating that the error was reduced by 54 % after considering the  $z_{0h}$  effect. The 288 result indicates that  $z_{0h}$  plays a critical role in both the SL scheme and the sensible heat flux (Chen and Zhang, 2009; Chen 289 et al., 2011). However, the error caused by Li of MM5 is still 6 % lowerlarger than that by of MM5Li. This illustrates that in 290 addition to the effect of roughness lengths, the algorithm of the Li scheme itself is more reasonable than that of MM5 scheme.

## 291 4.3 The specific performance of the two schemes in the severe haze pollution

There were two obvious pollution processes during this observation period and one occurred during December 13 to 23, 2016. Figure 7 shows the variations of hourly observed  $PM_{2.5}$  concentration as well as the momentum and sensible heat fluxes calculated by the Li and MM5 schemes at Gucheng station in this process. For the research purpose significance, only the daytime (from 8:00 a.m. to 20:00 p.m.) was taken into account. Note in MM5,  $z_0$  was 0.0419 when calculate momentum 296 fluxes and it was 0.0042 when calculate sensible heat fluxes. As shown in Fig. 7, the calculated results of momentum and 297 sensible heat fluxes forby the two schemes are generally consistent with the trend of the observations. Specifically, for the 298 momentum fluxes (Fig. 7a), the results of two schemes have little difference when the values of observed momentum fluxes 299 are large or at the peak. When the observed momentum fluxes are small, the Li-scheme results are close to or less than the 800 observations, while the MM5-scheme results are always higher than observations because of the limit of  $u_* = 0.1$  in this 301 scheme. For the sensible heat fluxes (Fig. 7b), MM5 results are always lower while Li results are closer to observations 302 especially when the observed values are small. Furthermore, according to the evolution of PM2.5 concentration, this haze event 303 was then divided into three stages: the clear stage (stage 1: 13~14), the transition stage (stage 2: 16~18) and the maintenance 304 stage (stage 3: 21~22). As shown in Fig. 7, in the clear stage (stage 1), the atmospheric stratification is unstable, PM<sub>2.5</sub> 305 concentration is low and there is a strong flux transport in the SL, the corresponding observations of the momentum and 306 sensible heat fluxes are relatively high and they vary greatly. In the transition stage (stage 2), the atmosphere is changing from 807 unstable to stable corresponding to haze formation, the momentum and sensible heat fluxes gradually decreases and the daily 308 variation also decreases. In the maintenance stage (stage 3), the atmospheric stratification is very stable, and flux transport in 309 the SL is weak, both the momentum and sensible heat fluxes are at a low level. It can be seen that the Li results are generally B10 closer to the observations compared comparing with MM5 results in all three stages.

B11 Figure 8 shows the probability distribution functions (PDF) of the difference between calculated fluxes (by using the Li 812 and MM5 schemes) and observations in different stages at Gucheng station. of momentum fluxes (Figs. 8a, 8c, 8e, 8g) and 813 sensible heat fluxes (Figs. 8b, 8d, 8f, 8h) calculated by using the Li and MM5 schemes in different stages at Gucheng station. B14 In the whole pollution process, for the momentum fluxes (Fig. 8a), the PDF of the difference by from Li tends to cluster in a B15 narrower range centered by 0, and the probability within  $\pm 0.005$  N m<sup>2</sup> is 46.82 %, while this value byfrom MM5 falls to 816 23.02 %. For the sensible heat fluxes (Fig. 8b), the PDF of the difference by from Li is also more concentrated around 0 than 817 that by from MM5. The probabilities of bias from by Li and MM5 within  $\pm 2.5$ W m<sup>2</sup> are 32.54 % and 13.49 %, respectively. In 818 stage 1, for the momentum fluxes (Fig. 8c), the probability of bias by from Li within  $\pm 0.005$  N m<sup>2</sup> is 38.09 %. The bias from of 319 MM5 mainly concentrates larger than 0, and the probability within  $\pm 0.005$ N m<sup>2</sup> is 14.29 %. For the sensible heat fluxes (Fig. 820 8d), the probability of Li-bias from Li within  $\pm 2.5$  W m<sup>2</sup> is 38.09 %, the same as momentum fluxes. The bias from of MM5 321 mainly concentrates less than 0, and the probability within  $\pm 2.5$  W m<sup>2</sup> is 9.52 %. In stage 2, the differences between the two B22 schemes are more obvious. The PDFsmomentum and sensible heat fluxes bias by from Li-is are the most concentrated around 823 0 in all cases, while the distribution of bias bythose from MM5 are is similar to that in stage 1. Specifically, for the momentum 824 fluxes (Fig. 8e), the probabilities of bias by from Li and MM5 within  $\pm 0.005$  N m<sup>2</sup> are 56.25 % and 25.00 %. For the sensible B25 heat fluxes (Fig. 8f), the values probabilities of bias by Li and MM5 within  $\pm 2.5$  W m<sup>2</sup> are 40.62 % and 6.25 %. In stage 3, the B26 difference between two schemes is small. For the momentum fluxes (Fig. 8g), the probabilities of bias byfrom Li and MM5

within  $\pm 0.005$  N m<sup>2</sup> are 22.73 % and 27.27 %. For the sensible heat fluxes (Fig. 8h), the <u>values probabilities of bias by from</u> Li and MM5 within  $\pm 2.5$  W m<sup>2</sup> are both 36.36 %.

829 Mean bias (MB), normalized mean bias (NMB), normalized mean error (NME) and root mean square error (RMES) of 830 Li and MM5 were calculated to test the results of two schemes. Table 2 shows that the Li scheme generally estimates better 331 than the MM5 scheme. In the whole haze process, the Li scheme underestimates the momentum fluxes by 3.63 % relative to 332 the observations, while the MM5 scheme overestimates by 34.03 %. The Li and MM5 schemes underestimate the sensible heat 333 fluxes by 15.69 % and 50.22 %, respectively. In the three stages, the Li scheme performs much better than the MM5 scheme 334 in the stage 1 and stage 2, especially in stage 2 when atmospheric stratification transforms from unstable to stable condition, 835 the difference between the Li and MM5 schemes areis particularly significant. That is, Tthe Li and MM5 schemes overestimate 836 the momentum fluxes by 7.68% and 45.56 %, respectively, while and Li and MM5they underestimate the sensible heat fluxes 837 by 33.84 % and 76.88 %. The error of Li is much less than that of MM5. Considering-In view of the importance role of 338 atmospheric stratification in the generation and accumulation of PM2.5 in stage 2, the Li scheme is expected to show better 339 performance in online simulation of PM<sub>2.5</sub> than MM5.

340 Based on the good behavior of the Li scheme in Gucheng, the same experiment was performed at Beijing station to discuss B41 the effect of different land-cover types on flux calculation-for two schemes. For Beijing station, the assumption  $z_{0m} = 1 \text{ m}$ , 342  $z_{0m}/z_{0h} = 10^6$  was made to represent the surface condition of megacity due to a lack in situ measurements of surface 343 turbulent flux. As shown in Fig. 9, the evolution of PM2.5 concentration at Beijing station was also divided into three stages B44 (stage 1: 13~15; stage 2: 17~19; stage 3: 20~21) just like Gucheng shown in Fig. 7 in the discussion. Compareing with Gucheng 845 to Fig. 7, there is a significant increase in the difference of momentum and sensible heat fluxes between Li and MM5 in Fig. 846 9. To be specific, the momentum transfer inat Beijing station is obviously larger than that in Gucheng due to the great increase 347 of the urban aerodynamic roughness length  $(z_{0m})$ . In the meanwhile, the difference between Li and MM5 has a further 348 expansion at Beijing station, compared with Gucheng. The sensible heat transfer byof the Li scheme has great difference 349 between clear days and pollution days, which is, the sensible heat transfer changes acutely in the stage 1 while it changes 850 smoothly in the stage 2 and stage 3. However, Tthe result sensible heat transfer by of the MM5 scheme is significantly different 851 compared from with Li result due to MM5 ignores the  $z_{0m}$  effect, and the small number of  $z_{0h}$  keeps the sensible heat 352 fluxes at a low level in all three stages.

To quantify the differences between the two schemes, a relative difference is defined in percentage:

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where  $V_{\text{Li}}$  and  $V_{\text{MM5}}$  are the momentum (or sensible heat) fluxes calculated by the Li and MM5 schemes, respectively. We obtained the relative differences at the two stations in the three stages through the statistics. It is clearly that the largest relative difference at Gucheng station is in the stage 2 and the valuethat at Beijing station is in the stage 1. The differences in Beijing

 $\Delta V = \left| \frac{V_{\rm Li} - V_{\rm MM5}}{V_{\rm MM5}} \right| \times 100 \ \%,$ 

(21)

are always larger than th<u>ose</u>at in Gucheng for each three stages. Specifically, the relative differences of momentum flux in stage 1, stage 2 and stage 3 increases by 73 %, 34 % and 27 %, respectively, and the results of sensible heat flux are 289 %, 52 % and 68 %, respectively.

We further <u>estimated the surface fluxes</u> <u>tested the two schemes</u> in whole Jing-Jin-Ji region <u>by using the two schemes</u>. Figure 10 shows the mean momentum and sensible heat fluxes calculated by Li and MM5 schemes and their differences in Jing-Jin-Ji during the pollution episode. The assumption  $(z_{0m} = 0.1 \text{ m}, z_{0m}/z_{0h} = 10^3)$  were <u>was</u> used to represent the average condition of the underlying surface of Jing-Jin-Ji region. As shown in Fig. 10, the momentum fluxes calculated by Li are less than <u>that those</u> by MM5 in most stations; the sensible heat fluxes calculated by Li are usually larger than <u>that those</u> by MM5. The result is consistent with the experiment <u>of at</u> Gucheng station, which further indicates the importance of considering <u>both</u>  $z_{0m}$  and  $z_{0h}$  <u>at the same time</u>.

## 368 5 Conclusions

369 Using the observed momentum and sensible heat fluxes, together with conventional meteorological data including 370 pressure, temperature, humidity and wind speed from December 1, 2016 to January 9, 2017, including a severe pollution 871 episode from December 13 to 23, 2016, the differences and the performance of between the Li and MM5 schemestwo surface schemes and the specific performances of the two were discussed and evaluated in this paper. The evolution process of 872 873 atmospheric stratification from unstable to stable corresponding to PM2.5 accumulationincreasing was mainly discussed. The 874 contributions of roughness lengths ( $z_{0m}$  and  $z_{0h}$ ) as well as other factors in the SL schemes to the momentum and sensible 875 heat flux\_flux\_calculation for the momentum and sensible heat were also discussed in details. The results are summarized as 376 follows:

1)  $z_{0m}$  and  $z_{0h}$  have important effects on turbulent flux calculation in the SL schemes. Different values of  $z_{0m}$  and  $z_{0h}$  in the schemes-could induce great changes in the flux calculation, indicating that it is very necessary and important to distinguish  $z_{0h}$  from  $z_{0m}$ . Ignoring the difference between the two in the MM5 scheme led to large errors in the calculation of sensible heat fluxes and this error in Gucheng iwas 54 %. Besides the roughness lengths, the algorithms-of two in schemes are also one of the important factors. In addition, ignoring the effect of the RSL in schemes may also result in certain bias of momentum and sensible heat fluxes in megacity regions which represent the rough underlying surface.

2) The effect of  $z_{0m}/z_{0h}$  on turbulent fluxes is closely related to land-cover types  $(z_{0m})$ . A rough land-cover type (large  $z_{0m}$ ) should be accompanied by a large value of  $z_{0m}/z_{0h}$ . The differences between the two schemes for ofthe momentum and sensible heat fluxes calculated by Li and MM5-in Beijing were much largerbigger in Beijing than thatose in Gucheng. This suggests that the MM5 scheme probably induces bigger greater error in megacities with rough surface (e.g., Beijing) than it-in

suburban area<u>s</u> with smooth surface (e.g., Gucheng) due to the irrational algorithm of MM5 scheme itself and the ignoring difference between  $z_{0m}$  and  $z_{0h}$ .

389 3) The Li scheme generally performed better than the MM5 scheme in the calculation of both the momentum flux and 890 the sensible heat flux-compared with observations at Gucheng station. The Li scheme made a better description in atmospheric 891 stratification which is closely related to the haze pollution, compared comparing with the MM5 scheme. This advantage was 392 the most prominent in the transition stage from unstable to stable atmospheric stratification corresponding to the PM2.5 393 accumulation. In this stage, the momentum flux calculated by Li was overestimated by 7.68 % and this overestimation by 394 MM5 was up to 45.56 %; the sensible heat flux by Li was underestimated by 33.84 % while this underestimation by MM5 was 895 even up to 76.88 %. In most Jing-Jin-Ji region, the momentum fluxes calculated by Li were less than thatose by MM5 and the 896 sensible heat fluxes by Li were larger than those the MM5, which was were consistent with Gucheng.

The offline study of the two SL schemes in this paper showed the superiority of the Li scheme for surface flux calculation corresponding to the  $PM_{2.5}$  evolution during the haze episode in Jing-Jin-Ji in eastern China. The study results offer the prerequisite and a possible way to improve PBL diffusion simulation and then  $PM_{2.5}$  prediction, which will be achieved in the follow-up work of <u>online</u>-integrating of the Li scheme into the atmosphere chemical models.

# 401 <u>Author contributions</u>

HW and YP conducted the study design. YL and CL provided the Li scheme and the flux data. CL helped with data
 processing. YP wrote the manuscript with help of HW and TZ. XZ, ZG, TJ, HC and MZ were involved in the scientific
 interpretation and discussion. All the authors commented on the paper.

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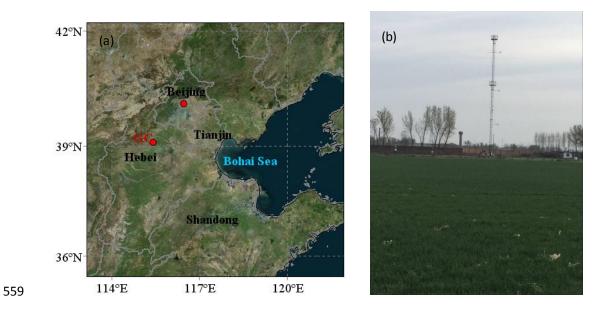
551	Table 1. Typical values of	$Z_{0m}$	corresponding to	o various land-cover types	s

z <sub>0m</sub> / m	Land-cover types		
5 ~ 50	Mountain (above 100m)		
1 ~ 5	The center of large cities, hills or mountain area		
0.1 ~ 1	Forests, the center of large towns		
0.01 ~ 0.1	Flat grasslands, agricultural fields		
$10^{-4} \sim 10^{-3}$	The snow surface, wide water surface, flat deserts		
10-5	The ice surface		

**Table 2.** Statistics between the Li and MM5 schemes calculated turbulent flux at Gucheng station.

		Li				MM5			
		MB	NMB	NME	RMSE	MB	NMB	NME	RMSE
Whole	τ	-0.0006	-3.63 %	54.29 %	0.0142	0.0058	34.03 %	63.59 %	0.0143
process	Н	-2.2723	-15.69 %	52.73 %	10.9649	-7.2735	-50.22 %	69.68 %	12.7946
Stage 1	τ	0.0021	9.98 %	55.90 %	0.0172	0.0091	43.45 %	66.66 %	0.0169
	Н	1.1775	5.79 %	37.87 %	10.5734	-7.1891	-35.34 %	55.70 %	13.1324
Stage 2	τ	0.0013	7.68 %	44.50 %	0.0111	0.0079	45.56 %	56.81 %	0.0121
	Н	-4.5752	-33.84 %	50.28 %	9.3995	-10.3924	-76.88 %	81.40 %	13.2553
Stage 3	τ	-0.0024	-13.25 %	59.13 %	0.0144	0.0030	16.72 %	56.34 %	0.0138
	Н	1.2818	11.39 %	66.31 %	11.4778	-1.7479	-15.52 %	65.90 %	10.4219

556 \*  $\tau$ : momentum flux; H: sensible heat flux; MB: mean bias; NMB: normalized mean bias; NME: normalized mean error; 557 RMSE: root mean square error. The units of MB and RMSE:  $\mu g m^{-3}$ .

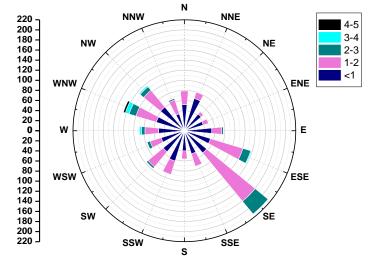


**Figure 1.** Location (a) and geographical environment (b) at Gucheng station. The map is from Bing Maps.

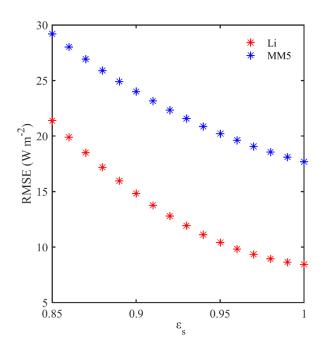




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**Figure 2.** Wind Rose map at Gucheng station from December 1, 2016 to January 9, 2017.



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571 Figure 3. The surface emissivity  $\varepsilon_s$  dependence of RMSE between observed near-neutral heat fluxes and parameterized heat 572 fluxes (red for Li and blue for MM5) at Gucheng station.

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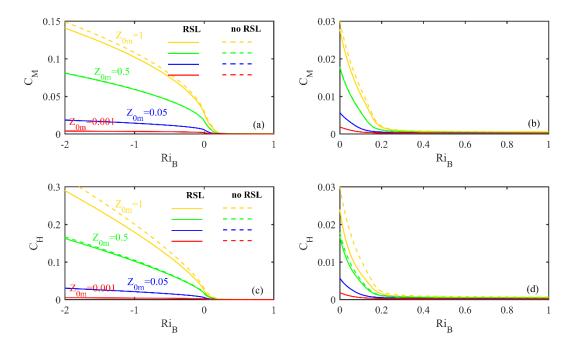
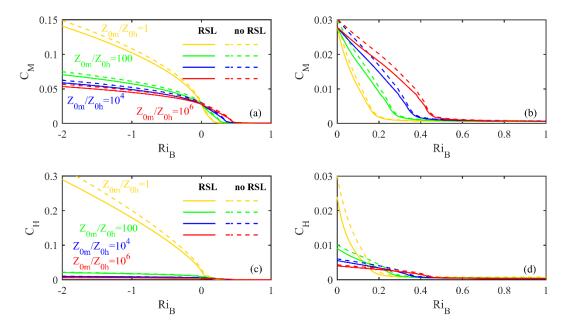
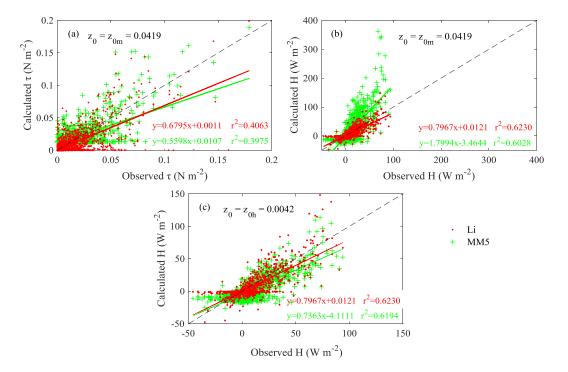


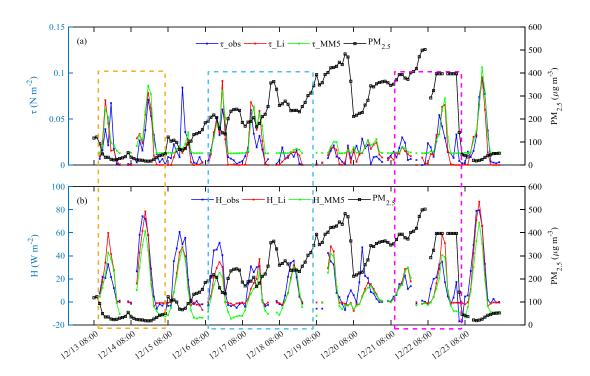
Figure 4. The relationships between  $C_M(C_H)$  and  $Ri_B$  for under different  $z_{0m}$  values and treatments of RSL. Solid lines: considering the RSL effect; dotted lines: without the RSL effect.



**Figure 5.** The relationships between  $C_M(C_H)$  and  $Ri_B$  for-under different ratios of  $z_{0m}$  to  $z_{0h}$  and treatments of RSL. Solid lines: considering the RSL effect; dotted lines: without the RSL effect.



**Figure 6.** Comparison of calculated and observed fluxes at Gucheng station from December 1, 2016 to January 9, 2017. (a) Momentum fluxes (MM5:  $z_0 = 0.0419$ ); (b) sensible heat fluxes (MM5:  $z_0 = 0.0419$ ); (c) sensible heat fluxes (MM5:  $z_0 = 0.0042$ ). Red dots: the Li scheme; green plus signs: the MM5 scheme.



**Figure 7.** Variations of hourly turbulent fluxes and observed  $PM_{2.5}$  at Gucheng station in daytime. (a) Momentum fluxes  $\tau$  (blue line: observations; red line: the Li scheme; green line: the MM5 scheme) and  $PM_{2.5}$  concentration (black line); (b) sensible heat fluxes H (the same as  $\tau$ ) and  $PM_{2.5}$  concentration (black line). Yellow box: stage 1; blue box: stage 2; purple box: stage 3. 599

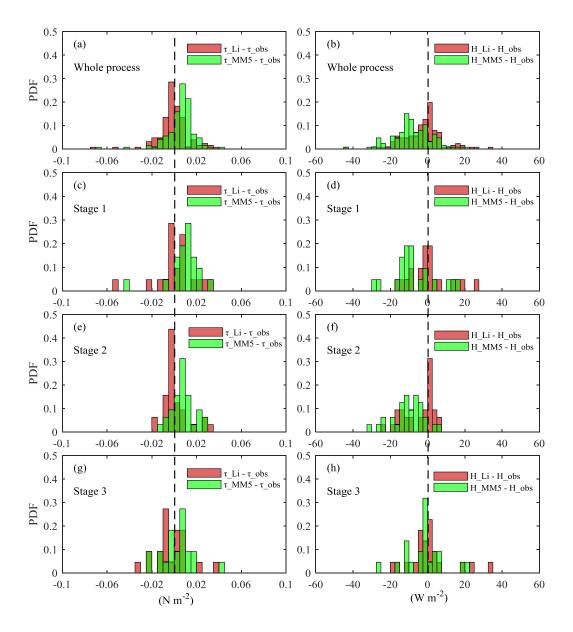
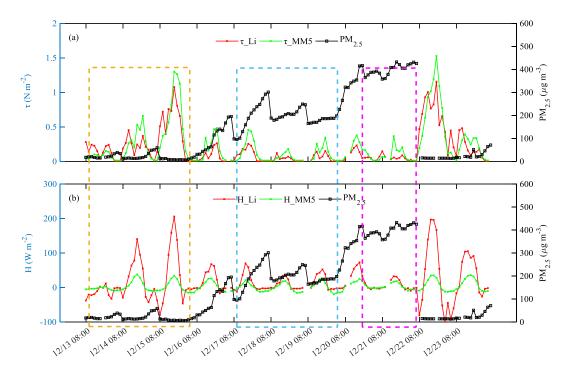
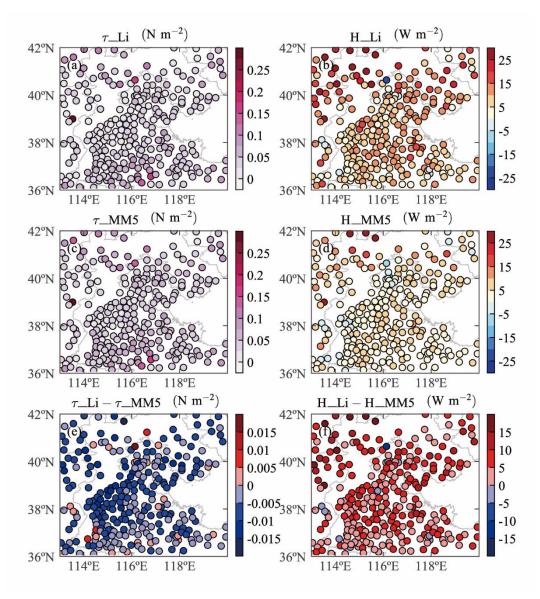


Figure 8. Probability distribution functions (PDF) of the differences between calculated fluxes (momentum fluxes: left;
sensible heat fluxes: right) by using two schemes (the Li scheme: red bars; the MM5 scheme: green bars) and observations in
different stages (a-b: whole process; c-d: stage 1; e-f: stage 2; g-h: stage 3).





**Figure 9.** As in Fig. 7 but for Beijing station.



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Figure 10. The mean momentum and sensible heat fluxes calculated by using two schemes (a-b: the Li scheme; c-d: the MM5
scheme) and their differences (Li minus MM5. e: difference of the momentum fluxes; f: difference of the sensible heat fluxes )

614 in Jing-Jin-Ji during the haze episode (December 13 to 23, 2016).