

Reply to Anonymous Referee #3:

We sincerely appreciate for the reviewer's careful dealing of our manuscript and valuable comments. We have read and discussed these comments in detail and answer them one by one in the followings. The corresponding revisions have also been added in the manuscript.

### **General comments by Referee #3**

*This study evaluated two surface layer schemes offline, and showed that the new Li scheme presents a better performance over the classic MM5 scheme in terms of the momentum and sensible heat fluxes. Given the importance of the surface exchange processes in a pollution episode and pollution forecast, an accurate representation of the surface processes would be required in a numerical model. This manuscript gave a rather good description about the two schemes, and the results did show that Li scheme may produce better agreement with observations especially in the transition stage of a haze episode.*

*However, I have a few major concerns about this paper:*

**Comment 1:** *What is the scientific contribution of this paper? The authors have well-addressed my comment in the quick report about the new improved surface layer scheme. However, as a scientific paper, I think the authors should also discuss and summarize the scientific findings of this study besides discussing the performance of the two schemes. For example,*

#### **Response:**

Thanks for the referee's advice. We have added some relevant content to strengthen the scientific contribution of our paper, and rewritten the conclusion and abstract of the manuscript. The scientific findings of this study are: (1)  $z_{0m}$  and  $z_{0h}$  have important effects on turbulent flux calculation in the SL schemes and ignoring the difference between  $z_{0m}$  and  $z_{0h}$  in the MM5 scheme could lead to large errors in calculation of sensible heat fluxes. In addition, ignoring the effect of the RSL in schemes may also results in certain bias of momentum and sensible heat fluxes in megacity regions which represent the rough underlying surface; (2) the magnitude of roughness lengths has significant influence on the two schemes. The difference of momentum and sensible heat fluxes calculated by Li and MM5 was much bigger over rough surface than over smooth surface, which suggests that the MM5 scheme probably induces bigger error in megacities with rough underlying surface than it in suburban area with smooth surface; (3) Li scheme better characterized the evolution of atmospheric stratification which is closely related to the haze pollution, compared with the MM5 scheme. This advantage was the most prominent in the transition stage from unstable to stable atmospheric stratification corresponding to the  $PM_{2.5}$  accumulation. The offline study of the two SL schemes in this paper showed the superiority of Li scheme for surface flux calculation corresponding to the  $PM_{2.5}$  evolution during the haze episode in Jing-Jin-Ji in east 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 online integrating of the Li scheme into the atmosphere chemical model.

**1) How does the roughness length affect the turbulent fluxes and hence the pollution?**

#### **Response:**

The surface parameters roughness lengths ( $z_{0m}$  and  $z_{0h}$ ) directly affect the calculation of both the surface layer scheme and the turbulent flux (momentum flux and sensible heat flux) which control the atmospheric stratification closely related to the haze pollution. To be specific, ignoring the difference between  $z_{0m}$  and  $z_{0h}$  in the MM5 scheme induced an obvious overestimation in calculating sensible heat flux (Fig. 6b). Instead, reasonable values of  $z_{0m}$  and  $z_{0h}$  in the Li scheme produced better agreement with observations (Figs. 6a-b). Furthermore, the Li scheme better characterized the evolution of atmospheric stratification from unstable to stable condition (Figs. 7-8), due to the reasonable treatment of the two parameters.

In addition, we added some new content to further discuss the important role of the roughness lengths (Figs. 9). The result showed that the differences of momentum and sensible heat fluxes calculated by Li and MM5 were much bigger in Beijing than that in Gucheng. This suggests that the MM5 scheme probably induces bigger error in megacities with rough surface (e.g., Beijing) than it in suburban area with smooth surface (e.g., Gucheng) due to the irrational algorithm of the MM5 scheme itself and the ignoring difference between  $z_{0m}$  and  $z_{0h}$ .

The study results above indicate the important role of the roughness lengths in turbulent fluxes and also suggest the

improving possibility of severe haze prediction in Jing-Jin-Ji in east China by coupling the Li scheme with more reasonable treatment of roughness lengths and algorithms into the atmosphere chemical model online.

2) *Does the roughness length plays a more important role in the transition stage of a pollution episode? And why?*

**Response:**

Yes. The Li scheme performed the best in the transition stage of the pollution episode at Gucheng station, compared with the MM5 scheme, and the biggest difference between Li and MM5 is the treatment of roughness lengths. Therefore, it can be inferred that the roughness lengths play a more important role in the transition stage of the pollution episode at Gucheng station. The results of Jing-Jin-Ji region were similar with Gucheng (Fig. 10 added in the revised manuscript).

In addition, we have added some new experiments to illustrate the important role of this surface parameter (Figs. 4-5, which were revised and add the contrast experiments of RSL). The results showed that the roughness lengths have a much higher effect on the momentum and sensible heat transfer than other factors such as the RSL as well as the universal function. We expect to find more observations to further evaluate it.

**Comment 2:** *There are a lot of grammar mistakes. Please carefully edit the manuscript to improve the language to ensure a better delivery of the scientific ideas and findings to the audience.*

**Response:**

We are so sorry for that. We have a careful examination of the full text including the tables and figures and revised the manuscript to ensure a better delivery of the scientific ideas and findings to the audience. All the changes can be seen in the manuscript with marked-up version.

Reply to Anonymous Referee #2:

We sincerely appreciate for the reviewer's careful dealing of our manuscript and valuable comments. We have read and discussed these comments in detail and answer them one by one in the followings. The corresponding revisions have also been added in the manuscript.

#### **General comments by Referee #2**

*This work evaluated the performance of a new surface layer scheme (Li) and a widely applied scheme (MM5) in simulating the momentum and sensible heat fluxes. Using the observational data in Gucheng station located in the southwest of Beijing from Dec 1, 2016, to Jan. 9, 2017, The authors found the Li scheme generally performed better than MM5 in calculating SL fluxes during the heavy pollution process. The study fits within the scope of the journal, and the manuscript is generally well written. The result presented is interesting as it shows the SL scheme performance in a polluted case. However, I found that some key details on the introductions are lacking and some of the discussions are not very well grounded.*

#### **Response:**

Thanks for the affirmation to our work. Yes, we agreed that some key points on the introduction were not enough and some discussions were not very well grounded. We have examined the introduction as well as whole text and the corresponding revisions have been added in the manuscript.

**Comment 1:** *The author should explicitly explain the scientific meaning of the paper. Since Li scheme has been published and evaluated in Li et al. (2014; 2015), why do we need additional evaluation using the observation during a severe haze episode from Gucheng station? I believe this evaluation may be necessary, but the authors need to illustrate clearly the specialty of this case. Also, the word "east China" appears several times in the paper. How did the author conclude Li generally performed better than MM5 in winter in east China since they only did one case in Beijing?*

#### **Response:**

The Li scheme consists of two parts (Li et al., 2014; 2015). The first part (Li et al., 2014) focused on the stable stratification, while the latter (Li et al., 2015) focused on the unstable conditions. The two parts have not been consolidated into a complete scheme in previous studies. In our study, the two parts were consolidated into one for both stable and unstable conditions. Furthermore, previous work (Li et al., 2014; 2015) was only compared with other iterative or non-iterative schemes. They have neither been compared with actual observations, nor evaluated under the transition process from unstable to stable conditions, which is essential and meaningful. We didn't introduce clearly in our old manuscript and we re-summarized this content in Line 74-83, Page 3 in the revised manuscript.

Yes, the word "east China" is not accurate in this paper. In fact, our study focuses on the Jing-Jin-Ji region in east China. We have replaced "east China" with "Jing-Jin-Ji" in the whole manuscript; In addition, we added Beijing station as well as Jing-Jin-Ji region to discuss the performance of Li and MM5 schemes for different land-cover types (added Figs. 9-10 and the related contents in the revised manuscript).

References:

1. Li, Y., Gao, Z., Li, D., Wang, L., and Wang, H.: An improved non-iterative surface layer flux scheme for atmospheric stable stratification conditions, *Geosci. Model Dev.*, 7, 515-529, <https://doi.org/10.5194/gmd-7-515-2014>, 2014.
2. Li, Y., Gao, Z., Li, D., Chen, F., Yang, Y., and Sun, L.: An Update of Non-iterative Solutions for Surface Fluxes Under Unstable Conditions, *Bound.-lay. Meteorol.*, 156, 501-511, <https://doi.org/10.1007/s10546-015-0032-x>, 2015.

**Comment 2:** *The role of surface layer (SL) scheme in air quality modeling needs to be further discussed in the introduction. The authors made sufficient introduction to the current status of SL. However, a detailed introduction of the importance of SL schemes in simulating pollution episode is somewhat lacking. In other words, the interactions between pollutant transportation, momentum and sensible heat (and how current SL schemes perform in momentum and sensible heat modeling) should be well established in the introduction part.*

#### **Response:**

We agree that the introduction of the interactions between pollutant transportation, momentum and sensible heat was

not enough and efficient, we read the new references list in the following and complemented the related contents in Line 42-52, Page 2 in the revised paper. The related references as follows were also added in the revised version.

References:

1. Zhang, R., Li, Q., and Zhang, R.: Meteorological conditions for the persistent severe fog and haze event over eastern China in January 2013, *Sci. China Earth Sci.*, 57, 26–35, <https://doi.org/10.1007/s11430-013-4774-3>, 2014.
2. Yang, Y., Liu, X., Qu, Y., Wang, J., An, J., Zhang, Y., and Zhang, F.: Formation mechanism of continuous extreme haze episodes in the megacity Beijing, China, in January 2013, *Atmos. Res.*, 155, 192–203, <https://doi.org/10.1016/j.atmosres.2014.11.023>, 2015.
3. Liu, T. T., Gong, S. L., He, J. J., Yu, M., Wang, Q. F., Li, H. R., Liu, W., Zhang, J., Li, L., Wang, X. G., Li, S. L., Lu, Y. L., Du, H. T., Wang, Y. Q., Zhou, C. H., Liu, H. L. and Zhao, Q. C.: Attributions of meteorological and emission factors to the 2015 winter severe haze pollution episodes in China's Jing-Jin-Ji area, *Atmos. Chem. Phys.*, 17, 2971–2980, <https://doi.org/10.5194/acp-17-2971-2017>, 2017.
4. Zhong, J., Zhang, X., Dong, Y., Wang, Y., Liu, C., Wang, J., Zhang, Y., and Che, H.: Feedback effects of boundary-layer meteorological factors on cumulative explosive growth of PM<sub>2.5</sub> during winter heavy pollution episodes in Beijing from 2013 to 2016, *Atmos. Chem. Phys.*, 18, 247–258, <https://doi.org/10.5194/acp-18-247-2018>, 2018.
5. Li, Z., Guo, J., Ding, A., Liao, H., Liu, J., Sun, Y., Wang, T., Xue, H., Zhang, H., and Zhu, B.: Aerosol and boundary-layer interactions and impact on air quality, *Natl. Sci. Rev.*, 4, 810–833, <https://doi.org/10.1093/nsr/nwx117>, 2017.
6. Li, T., Wang, H., Zhao, T., Xue, M., Wang, Y., Che, H., and Jiang, C.: The Impacts of Different PBL Schemes on the Simulation of PM<sub>2.5</sub> during Severe Haze Episodes in the Jing-Jin-Ji Region and Its Surroundings in China, *Adu. Meteorol.*, <http://dx.doi.org/10.1155/2016/6295878>, 2016a.
7. Vautard, R., Moran, M. D., Solazzo, E., Gilliam, R. C., Matthias, V., Bianconi, R., Chemel, C., Ferreira, J., Geyer, B., Hansen, A. B., Jericevic, A., Prank, M., Segers, A., Silver, J. D., Werhahn, J., Eolke, R., Rao, S. T., and Galmarini, S.: Evaluation of the meteorological forcing used for the Air Quality Model Evaluation International Initiative (AQMEII) air quality simulations, *Atmos. Environ.*, 53, 15-37, <https://doi.org/10.1016/j.atmosenv.2011.10.065>, 2012.

**Comment 3:** *In the third conclusion (Line 342-343): The authors argued that “During the heavy pollution process, the calculated momentum and sensible heat fluxes by the Li scheme were better than those by the MM5 scheme generally”. If the authors only compared simulated momentum and sensible heat to the observation, why this work emphasized the “heavily polluted conditions”? Future work may consider coupling SL scheme with atmospheric chemistry models to compare the modeled pollutant concentration with observation directly.*

**Response:**

The statement “During the heavy pollution process, the calculated momentum and sensible heat fluxes by the Li scheme were better than those by the MM5 scheme generally” was inaccurate. In fact, the surface turbulent flux affects the stability of atmospheric stratification directly, which further influences the air pollution. The little turbulence flux transfer corresponds to stable atmospheric stratification and which may lead to the heavy pollution. In order to make our meaning clearly, we have rewritten this part in Line 377-384, Page 13 in the revised paper.

Thanks for the referee's kind advice. We are online coupling the new scheme into atmosphere chemical models to compare the modeled pollutant concentration with observation directly and the related results will be discussed in next paper.

**Minor comments:**

**Comment 1:** *Line 65-66: Why is the pollution episode important? The author may need to specify and add more discussion instead of arguing “few studies discussed it based on a pollution episode corresponding various atmospheric states”.*

**Response:**

Yes, this part was not clearly described. We read some new references (list in the following) and add the related content to explain why the pollution episode is important in Line 76-83, Page 3, instead of “few studies discussed it based on a pollution episode corresponding to various atmospheric states”.

References:

1. Wang, H., Tan, S. C., Wang, Y., Jiang, C., Shi, G., Zhang, M., and Che, H. Z.: A multisource observation study of the severe prolonged regional haze episode over eastern China in January 2013, *Atmos. Environ.*, 89, 807-815, <https://doi.org/10.1016/j.atmosenv.2014.03.004>, 2014.
2. Zhang, B., Wang, Y., and Hao, J.: Simulating aerosol-radiationcloud feedbacks on meteorology and air quality over eastern China under severe haze conditions in winter, *Atmos. Chem. Phys.*, 15, 2387–2404, <http://doi.org/10.5194/acp-15-2387-2015>, 2015.
3. Li, T., Wang, H., Zhao, T., Xue, M., Wang, Y., Che, H., and Jiang, C.: The Impacts of Different PBL Schemes on the Simulation of PM<sub>2.5</sub> during Severe Haze Episodes in the Jing-Jin-Ji Region and Its Surroundings in China, *Adu. Meteorol.*, <http://dx.doi.org/10.1155/2016/6295878>, 2016a.
4. Liu, T. T., Gong, S. L., He, J. J., Yu, M., Wang, Q. F., Li, H. R., Liu, W., Zhang, J., Li, L., Wang, X. G., Li, S. L., Lu, Y. L., Du, H. T., Wang, Y. Q., Zhou, C. H., Liu, H. L. and Zhao, Q. C.: Attributions of meteorological and emission factors to the 2015 winter severe haze pollution episodes in China's Jing-Jin-Ji area, *Atmos. Chem. Phys.*, 17, 2971–2980, <https://doi.org/10.5194/acp-17-2971-2017>, 2017.

**Comment 2:** *Line 172-180: The observation and method should be introduced in further details. What is the spatial representativeness of the station? Can it represent the whole east China? If not, should add more cases in other parts of China or considering changing this word. What is the measuring height for the fluxes? (Could refer to Liu et al. 2016 as an example for the introduction)*

**Response:**

This suggestion is very valuable and we revised the manuscript as following according to this suggestion and the recommended reference.

We have added some introduce about the observation and method in details. Please see Line 183-202, Page 7. The measuring height for the fluxes in Gucheng station is 4 m, which is added in Line 188, Page 7.

Gucheng station is a farmland site where rice is planted in summer and wheat in winter, its surroundings are mainly farmland and scattered villages which represents suburban with smooth surface and it does not represent the whole east China. In fact, our study focuses on “Jing-Jin-Ji” region in east China. We changed “east China” as “Jing-Jin-Ji” in the manuscript; According to the referee’s comment, the similar experiment and discussion at Beijing station which represents megacity with rough surface, were added in the revised manuscript (Fig. 9), and the difference of the two schemes in Jing-Jin-Ji region (Fig. 10) was also added in the manuscript.

**Comment 3:** *Line 182-189: The data processing should be explained in further details and add more reference in data processing methods (Line 182-Line 189). For example, how was the quality control conducted? The reference for quality control may be included if they have been applied in the study (e.g., frequency response correction (Moore, 1986) and WPL correction (Webb et al., 1980), or quality control (Foken et al., 2004)).*

**Response:**

Thanks very much for the references recommended by the referee. We have read these references and explained the data processing in more details (Line 196-202, Page 7) and added the relevant reference in Line 197, Page 7.

**Comment 4:** *Please explain why  $z = 10\text{ m}$  has been used (line 218)?*

**Response:**

“Considering the lowest level in mesoscale models is usually about 10m,  $z = 10\text{ m}$  is set as the reference height.” The revised part can be found in Line 244, Page 9.

**Comment 5:** *What variables have been used in Li and MM5 schemes? In the third part (Observational data and methods), the paper only introduced the data acquired from the Gucheng station, without specifying what variables would be used in the two schemes.*

**Response:**

Both Li and MM5 schemes use same variables acquired from Gucheng and other stations. The variables used in the two schemes were add in the paper “The measured meteorological variables including wind speed and direction, temperature, humidity, pressure, radiation are used to calculate the momentum and sensible heat fluxes both in the Li and MM5 schemes.” The new revision can be seen in Line 189-191, Page7.

**Comment 6:** *Straight from 5. Line 247, the authors mentioned: “Given the observational data, a dataset of Z0m (Z0h) then is generated”. What variables were used in calculating Z0m and Z0h? This may be clarified in the third part (observational data and methods).*

**Response:**

The specific variables are added including pressure, temperature, humidity, wind speed and direction, flux for momentum and sensible heat at 4m height, surface skin temperature and we moved this part to the Section 3.3 (Determination of roughness length  $z_{0m}$  ( $z_{0h}$ )) according to the referee’s suggestion. The revised details can be found in Line 214-223, Page 8.

**Comment 7:** *Line 250 to Line 264: The author may consider comparing their conclusion with analysis from other papers (Chen et al. 2009; Chen et al. 2011). The reference used here is somewhat out of date.*

**Response:**

This part (Section 4.3) mainly compared the Li and MM5 schemes in flux calculation during observation. We have not any references in this section, so we are not sure which reference used here is somewhat out of date. However, we read the two papers and added the two references in our manuscript (Line 282-283, Page 10) for the related content with our study.

**Comment 8:** *In the Fig. 4, the authors showed the effect of the roughness length on flux calculation by choosing different  $z_{0m}$  values. Since the  $z_{0m}$  and  $z_{0h}$  has already been determined in the crop field, I feel it may not be necessary to discuss the influence of roughness length on the calculation of turbulent flux.*

**Response:**

$z_{0m}$  is mainly determined by land-cover type and canopy height, but  $z_{0h}$  is also affected by nature of the atmospheric flow (Brutsaert, 1975), the underlying surface is neither the only one, nor the most important factor for  $z_{0h}$ . Furthermore, the different treatment of  $z_{0m}$  and  $z_{0h}$  in different schemes (e.g., Li and MM5) has great impact on flux calculation and this is also the main reason why the Li scheme is superior to MM5 discussed in the manuscript (Figs. 5, 7, and 8). Therefore, it is necessary and important to discuss the effects of  $z_{0m}$  and  $z_{0h}$  on the calculation of turbulent flux.

Reference: Brutsaert, W., The roughness length for water vapor, sensible heat, and other scalars, J. Atmos. Sci., 32, 2028 – 2031, 1975.

**Comment 9:** *Line 315-316: In the previous results and discussion, the authors only analyzed the superiority of Li scheme in modeling sensible heat and momentum flux. More analysis is needed discussing the SL flux influence the air pollution process should be illustrated before concluding “the superiority of Li scheme in the air pollution modeling.”*

**Response:**

The expression of the paragraph “Therefore, the superiority of the Li scheme in the air pollution process, especially in this stage is of great reference value for improving the forecast of pollutant concentration in the current air quality model. In stage 3, the difference between the two schemes is not obvious” is not clear enough. Offline study of the two schemes in this work could not draw the conclusion “the superiority of Li scheme in the air pollution modeling”, but it is expected to better performance in online simulation of  $PM_{2.5}$  based on its obvious superiority in the offline study results. So, this paragraph was replaced by “The error of Li is much less than that of MM5. Considering the importance of atmospheric stratification in the generation and accumulation of  $PM_{2.5}$  in stage 2, the Li scheme is expected to show better performance in online simulation of  $PM_{2.5}$  than MM5.” The details can be found in Line 330-332, Page 12 in the revised paper.

Please note that all revised manuscript mentioned above is the final clean manuscript version.

# The evaluating study of the momentum and heat exchange process of two surface layer schemes during the severe haze pollution in Jing-Jin-Ji in east China

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**Abstract.** The turbulent flux parameterization schemes in surface layer are crucial for air pollution modeling. The pollutants prediction by atmosphere chemical model exist obvious deficiencies, which may be closely related to the uncertainties of the momentum and sensible heat fluxes ~~calculation~~calculated in the surface layer. The differences of two surface layer schemes (the Li and MM5 scheme) were discussed and the performance of the two schemes was evaluated based on the observed momentum and sensible heat fluxes in Jing-Jin-Ji in east China.In this study, a new surface layer scheme (Li) and a classic scheme (MM5) were compared and evaluated based on the observed momentum and sensible heat fluxes in east China during a severe haze episode in winter. The results showed that the aerodynamic roughness length  $z_{0m}$  and the thermal roughness length  $z_{0h}$  play an important role in the flux calculation, it is necessary to distinguish the thermal roughness length  $z_{0h}$  from the aerodynamic roughness length  $z_{0m}$ , and ignoring the difference between the two led to large errors of the momentum and sensible heat fluxes in MM5. Compared with the Li scheme, ignoring the difference between the two in the MM5 scheme induced great 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 as well as the roughness sublayer also resulted in certain errors in the MM5 scheme. In addition, the magnitudes of  $z_{0m}$  and  $z_{0h}$  have significant influence on the two schemes. The large  $z_{0m}$  and  $z_{0m}/z_{0h}$  in megacity with rough surface (e.g., Beijing) resulted in much larger differences of momentum and sensible heat fluxes by Li and MM5, compared with the small  $z_{0m}$  and  $z_{0m}/z_{0h}$  in suburban area with smooth surface (e.g., Gucheng). The error of calculated sensible heat flux was reduced by 54% after discriminating  $z_{0h}$  from  $z_{0m}$  in MM5.

Besides, the algorithm itself of Li scheme performed generally better than MM5 in winter in east China and the momentum flux bias of the Li scheme was lower about 12%, sensible heat flux bias about 5% than those of MM5 scheme. Most of all, the Li scheme better characterized the evolution of atmospheric stratification than the MM5 scheme in general, especially showed a significant advantage over MM5 for the transition stage from unstable to stable atmospheric stratification corresponding to the PM<sub>2.5</sub> accumulation. The bias of momentum and sensible heat fluxes bias of Li were lower about 38% and 43% respectively than those from MM5 during this stage, sensible heat flux bias about 43% than those of MM5 during the PM<sub>2.5</sub> increasing stage. This study result indicates the ability superiority of the Li scheme for more accurate in the describing of the regional atmospheric stratification, and also suggests the potential-improving possibilities of severe haze prediction in Jing-Jin-Ji in east China by online-coupling it into the atmosphere chemical model online.

**Key words:** surface layer; turbulent flux parameterization; roughness length; numerical modeling; air pollution

## 1 Introduction

Adequate air quality modeling relies on accurate simulations of meteorological conditions, especially in planetary boundary layer (PBL) (Hu et al., 2010; Cheng et al., 2012; Xie et al., 2012). The PBL is closely coupled to the earth's surface by turbulent exchange processes. As the bottom layer of PBL, the surface layer (SL) close to the earth's surface reflects the surface state by calculating momentum, heat, water vapor and other fluxes, and influences the atmospheric structure by turbulent transport process. Many studies have illustrated the important roles of meteorological factors in the SL in the formation of air pollution. They demonstrated that weak wind speed, high relative humidity (RH) and strong temperature inversion are favorable for the haze concentrating (Zhang et al., 2014; Yang et al., 2015; Liu et al., 2017; Zhong et al., 2017). The strong stable stratification and weak turbulent are mainly responsible for many haze events. The relationship between flux and atmospheric profile in the atmospheric surface layer is a key factor for air pollution diffusion, especially under stable stratification conditions (Li et al., 2017). However, the study of stable boundary layer still has some uncertainties due to the poor description of surface turbulent motion. The simulating study on a severe haze in east China by the Weather Research and Forecasting/Chemistry (WRF-Chem) model concluded that there is lower ability of current PBL schemes in distinguishing the diffusion between haze days under stable condition and clean days under unstable condition (Li et al., 2016a). Another study (Vautard et al. 2012) on mesoscale meteorological models also pointed out a systematic overestimation of near-surface wind speed in a stable boundary layer and its possible contribution to the underestimation of the PM<sub>2.5</sub> pollution. The SL provides important bottom boundary conditions, as the bottom layer of the PBL. In addition, atmospheric conditions in both the PBL and upper layers are strongly dependent on the turbulent fluxes which are computed in the SL (Ban et al., 2010). Flux parameterization in the SL plays an important role in studies of the hydrological cycle and weather prediction (Yang et al., 2001; Li et al., 2014). An adequate SL scheme is crucial to provide an accurate atmospheric



65 evolution by numerical models (Jiménez et al., 2012) and hence it may introduce important impacts on air pollution  
66 simulation.

67 ~~In many numerical models, surface momentum, heat and moisture fluxes calculated by a SL scheme are coupled to a~~  
68 ~~Land Surface Module, which in turn provides input to the PBL module. Therefore, an adequate SL scheme is crucial for the~~  
69 ~~model performance (Jiménez et al., 2012). It was reported that the difference of 2 m temperature modeling in three PBL~~  
70 ~~schemes is due to different calculation of sensible heat fluxes in the SL (Hu et al., 2010). Tymvios et al.(2017) evaluated the~~  
71 ~~performance of Weather Research and Forecasting (WRF) model with a combination of several PBL and compatible SL~~  
72 ~~schemes and emphasized the importance of SL schemes.~~

73 ~~The bulk aerodynamic formulation~~Most SL schemes used in numerical models are bulk algorithms which are based on  
74 Monin-Obukhov similarity theory (hereinafter MOST, Monin and Obukhov, 1954) is usually employed to calculate surface  
75 fluxes in numerical models. ~~In a bulk algorithm, vertical fluxes in the SL can be considered constant. The effects of shear~~  
76 ~~stress and buoyancy on turbulent transport are discussed with the method of similarity theory and dimensional analysis.~~  
77 Turbulent fluxes ~~in models~~ are parameterized by wind, temperature, ~~humidity~~moisture in the lowest layer in model and  
78 temperature and humidity in surface, ~~surface skin temperature and humidity.~~ Many international scholars verified the MOST  
79 using of field experiments and then proposed the universal functions, the commonly used of which is Businger-Dyer (BD)  
80 equation (Businger, 1966; Dyer, 1967). With the development of observation technology, the coefficients in the BD equation  
81 have been further modified (e.g., Paulson, 1970; Webb, 1970; Businger et al., 1971; Dyer, 1974; Högström, 1996). In  
82 addition to the BD equation, some other schemes have been put forward and they ~~may~~ performed better especially for the  
83 strongly stable stratification (e.g., Holtslag and De Bruin, 1988; Beljaars and Holtslag, 1991; Cheng and Brutsaert, 2005).  
84 The schemes can be divided into two types according to the computing characteristics. One type is called as iterative  
85 algorithm (e.g., Paulson, 1970; Businger et al., 1971; Dyer, 1974; Högström, 1996; Beljaars and Holtslag, 1991), and it  
86 keeps the MOST completely with less approximation so that the results can be more precise. However, it needs to take much  
87 more steps to converge and hence the CPU time is consuming which reduces the computational~~affects the ability and~~  
88 ~~efficiency of modeling (Louis, 1979; Li et al., 2014); The other one is called as non-iterative algorithm (e.g., Louis et al.,~~  
89 ~~1982; Launiainen, 1995; Wang et al., 2002; Wouters et al., 2012). Due to the approximate treatment, there is no need for~~  
90 ~~loop iteration in the calculation due to the approximate treatment. This algorithm~~ is much simpler and less CPU  
91 time-consuming, but the results are based on the loss of the calculation accuracy.~~it may lead to a lower accuracy of the~~  
92 ~~results.~~

93 ~~Although many researches above focused on the effects of the SL schemes on PBL and meteorological elements, few~~  
94 ~~studies discussed it based on a pollution episode corresponding various atmospheric states. The turbulent exchange of~~  
95 ~~momentum, heat, and moisture at the ground surface is more important than large scale transport for the accumulation and~~

transport of pollutants when atmosphere is stable. In this paper, two kinds of surface flux calculation schemes were compared and evaluated during a haze episode using observational flux data. One is a new ~~A new non-iterative~~ scheme proposed by Li et al. (2014; 2015, Li hereinafter), ~~speeds up effectively under a higher accuracy compared with some classic iterative computation.~~ It is remarkable that this new scheme just have been theoretically evaluated and it has never been applied in any models. Haze pollution occurs frequently in recent years in east China. The concentration of  $PM_{2.5}$  may reach up to  $1000 \mu\text{g} \cdot \text{m}^{-3}$  in the Beijing-Tianjin-Hebei (Jing-Jin-Ji) region in winter (Wang et al., 2014) while it was generally underestimated by current air quality models (Zhang et al., 2015; Li et al., 2016a; Liu et al., 2017). The Li and another classic SL scheme (Zhang and Anthes, 1982, MM5 hereinafter) are compared in details in this study, ~~the other is MM5 similarity~~ The observed momentum and sensible heat flux data covering once complete haze process at Gucheng station was used to evaluate the two schemes focusing on the transition stage from unstable to stable atmospheric stratification corresponding to the  $PM_{2.5}$  accumulation. The evaluation is in the view of both local and regional scales. This offline study may provide the prerequisite for the online coupling the Li scheme into atmosphere chemical model in the future, ~~scheme~~ (Zhang and Anthes, 1982, MM5 hereinafter) which is widely applied in modeling investigation (e.g., Hu et al., 2010; Wang et al., 2015a, b; Tymvios et al., 2017). As a new one, the Li scheme is not yet applied to the atmosphere chemical models, and few relevant articles evaluate this scheme using the observational data especially in a haze episode. In this scheme, the aerodynamic roughness length  $z_{0m}$  and thermal roughness length  $z_{0h}$  are distinguished each other and the effect of the roughness sublayer (RSL) is taken into account. In addition, this scheme can be applied to the full range of roughness status  $10 \leq \frac{z}{z_{0m}} \leq 10^5$  and  $0.5 \leq \ln \frac{z_{0m}}{z_{0h}} \leq 30$  under whole conditions  $-5 \leq Ri_B \leq 2.5$ . Here  $z$  is the reference height and  $Ri_B$  is the bulk Richardson number. Compared with Li, the MM5 scheme does not consider the effect of both  $z_{0h}$  and the RSL. Further, in order to keep the stability of modeling, some limits have been used in MM5 such as a limit of 10 is used for both the stability parameter  $\zeta$  and universal functions.

## 2 Theory

The definition of the momentum and sensible heat flux ~~are introduced, and as well as~~ the detailed algorithms of the Li and MM5 schemes are ~~explained~~ introduced in this section.

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

The turbulent fluxes from ground surface are defined as follows:

$$\tau = \rho u_*^2 \quad \text{and} \quad (1a)$$

$$H = -\rho c_p u_* \theta_* \quad (1b)$$

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

125 constant pressure.  $u_*$  and  $\theta_*$  are the friction velocity and the temperature scale, respectively, and they represent the  
 126 intensity of the vertical turbulent flux transport and they are approximately independent on height in the SL.

127 Both the Li and MM5 schemes are calculated with bulk flux parameterization. As an important dimensionless parameter  
 128 related with the stability, the bulk Richardson number  $Ri_B$  is defined as

$$129 Ri_B = \frac{gz(\theta - \theta_g)}{\theta u^2}. \quad (2)$$

130 Where  $g$  is the acceleration of gravity,  $z$  is the reference height which is the lowest level in the model,  $\theta$  is the mean  
 131 potential temperature at height  $z$ ,  $\theta_g$  is the surface radiometric potential temperature,  $u$  is the mean wind speed at height  $z$ .

132 Thus,  $Ri_B$  can be computed through meteorological data at least two levels.

## 133 2.2 The Li scheme

134 ~~This new scheme employ non-iterative algorithm to compute the surface fluxes. The~~ basic idea ~~of Li~~ is to  
 135 parameterize ~~the stability parameter~~  $\zeta$  directly with  $Ri_B$  ~~and roughness lengths~~ ( $-z_{0m}$  and  $z_{0h}$ ). ~~Specifically and then~~  
 136 ~~calculate turbulence fluxes. In the scheme~~, bulk transfer coefficients of the momentum and sensible heat fluxes ( $C_M$  ~~and~~  $C_H$ )  
 137 are expressed as

$$138 C_M = \frac{u_*^2}{u^2} = \frac{\tau}{\rho u^2}, \quad \text{and} \quad (3a)$$

$$139 C_H = \frac{u_* \theta_*}{u(\theta - \theta_g)} = -\frac{H}{\rho c_p u(\theta - \theta_g)}. \quad (3b)$$

140 Based on MOST and considering the RSL effect ~~at the same time~~, the relationship between the bulk transfer coefficients  
 141 and the profile functions corresponding to wind and potential temperature are usually expressed as

$$142 C_M = \frac{k^2}{\left[ \ln \frac{z}{z_{0m}} - \psi_M \left( \frac{z}{L} \right) + \psi_M \left( \frac{z_{0m}}{L} \right) + \psi_M^* \left( \frac{z}{L}, \frac{z}{z_*} \right) \right]^2}, \quad \text{and} \quad (4a)$$

$$143 C_H = \frac{k^2}{R \left[ \ln \frac{z}{z_{0m}} - \psi_M \left( \frac{z}{L} \right) + \psi_M \left( \frac{z_{0m}}{L} \right) + \psi_M^* \left( \frac{z}{L}, \frac{z}{z_*} \right) \right] \left[ \ln \frac{z}{z_{0h}} - \psi_H \left( \frac{z}{L} \right) + \psi_H \left( \frac{z_{0h}}{L} \right) + \psi_H^* \left( \frac{z}{L}, \frac{z}{z_*} \right) \right]}. \quad (4b)$$

144 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~~  
 145 two schemes,  ~~$-z_{0m}$  and  $z_{0h}$  are the aerodynamic roughness length and the thermal roughness length, respectively.~~  $\psi_M$  and

146  $\psi_H$  are the integrated stability functions for momentum and sensible heat, respectively, which are also called universe  
 147 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

148 ~~height of RSL height. It is clear to~~ ~~From above equations we can~~ see that the calculation of the momentum and sensible heat  
 149 flux requires  $C_M$  and  $C_H$  (or  $u_*$  and  $\theta_*$ ), and there are 3 key points to get them:

- 150 1.  $z_{0m}$  and  $z_{0h}$ .  $z_{0m}$  and  $z_{0h}$  are two key parameters in the bulk transfer equations, ~~and~~ ~~†~~ Their definitions and  
 151 influence will be ~~discussed given~~ in Sect. 4.1. ~~Note that both  $z_{0m}$  and  $z_{0h}$  are taken into account by the Li scheme. In~~  
 152 ~~other words, the Li scheme distinguishes these two important surface parameters effectively as they generate from~~  
 153 ~~different mechanisms.~~

2.  $\zeta$ . ~~In the Li scheme, the~~ determination of  $\zeta$  is the most crucial problem for ~~the Li scheme. In fact, this new~~ ~~scheme includes two parts. The first part was proposed for atmospheric stable stratification condition (Li et al., 2014),~~ ~~and the second part then extended the scheme to unstable condition (Li et al., 2015). For stable condition~~ ~~calculation of~~ ~~turbulent fluxes. Li is a new scheme based on the results of Yang et al. (2001), Wouters et al. (2012), Sharan and~~ ~~Srivastava (2014), and which is proposed to approach the classic iterative computation results using multiple~~ ~~regressions. In particular, under 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  $z_{0h}$  ~~with Table 1 (see Li et al., 2014);~~ (2) find the section according to the region and  $Ri_B$  with Eq. (5) and ~~given~~ coefficients ~~in Table 2 (see Li et al., 2014);~~ (3) calculate  $\zeta$  ~~using~~ Eq. (6) and ~~given coefficients. Tables 3-10 (see Li et al., 2014).~~

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

$$\zeta = Ri_B \sum C_{ijk} Ri_B^i L_{0M}^j (L_{0H} - L_{0M})^k. \quad (6)$$

Where  $C_{mn}$  and  $C_{ijk}$  are the coefficients in Tables ~~in Li et al. (2014)~~ ~~3-10~~.  $L_{0M} = \ln \frac{z}{z_{0m}}$ ,  $L_{0H} = \ln \frac{z}{z_{0h}}$ .  $m, n = 0, 1, 2$ , and  $m + n \leq 3$ ;  $i, j, k = 0, 1, 2, 3$ , and  $i + j + k \leq 4$ . Similarly, ~~under~~ ~~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:

$$\zeta = Ri_B \frac{L_{0M}^2}{L_{0H}} \sum C_{ijk} \left( \frac{-Ri_B}{1-Ri_B} \right)^i L_{0M}^{-j} L_{0H}^{-k}. \quad (7)$$

Where  $C_{ijk}$  is ~~is listed in Li et al. (2016)~~ ~~seen in Table 2 (Li et al., 2016)~~, and  $i = 0, 1$ ;  $j, k = 0, 1, 2, 3$ ;  $i + j + k \leq 4$ .

3. Universal function. It is also a key factor in flux calculation. The form of universal function is adopted from ~~CB05~~ ~~(Chenge and Brutsaert, (2005) under the stable condition (Eqs. (8a), (8b)) and Paulson\_70 (Paulson, (1970) under the~~ ~~unstable condition (Eqs. (9a), (9b)):~~

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

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

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

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

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

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. 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 the RSL effect in the calculation~~

of turbulent fluxes, especially for the rough terrain such as forest or large cities. Ridder (2010) proposed the expression of  $\psi_M^*$  and  $\psi_H^*$ :

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

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

Where  $v = 0.5$ ,  $\mu_M = 2.59$ ,  $\mu_H = 0.95$ ,  $z_* = 16.7 z_{0m}$ ,  $\lambda = 1.5$ .  $\phi_M$  and  $\phi_H$  are universal functions before integration. Here, set  $\chi_M = 1 + \frac{v}{\mu_M z / z_*}$ ,  $\chi_H = 1 + \frac{v}{\mu_H z / z_*}$ :

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

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

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

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

~~The Li scheme is summarized as: firstly determine  $Ri_B$ ,  $z_{0m}$  and  $z_{0H}$  according to the observation data, and then calculate  $\zeta$  with  $Ri_B$ ,  $z_{0m}$  and  $z_{0H}$ . Finally carry out the momentum and sensible heat fluxes under different stratification conditions.~~

### 2.3 The MM5 scheme

~~The MM5 scheme is a classic one which is widely applied in modeling investigation (Hu et al., 2010; Wang et al., 2015a, b; Tymvios et al., 2017). This scheme dose not distinguish  $z_{0h}$  from  $z_{0m}$ , thus the roughness length here is expressed as  $z_0$ . For unstable condition, Eqs. (16a) and (16b) give the function forms following Paulson (1970), and for stable condition, the atmospheric stratification conditions are subdivided into three cases according to Zhang and Anthes (1982) and the function forms are given by Eqs. (13), (14), and (15). In this scheme, no distinction is made between  $z_{0m}$  and  $z_{0H}$ , thus we express the roughness length with  $z_0$ . Under the unstable condition, take Paulson70 with Eqs. (16a) and (16b), and under the stable condition, the atmospheric stratification conditions are subdivided into three cases according to Zhang and Anthes (1982). In addition, this scheme does not consider the RSL effect.~~

(1) Strongly stable condition ( $Ri_B \geq 0.2$ ):

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

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

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

(3) Neutral condition ( $Ri_B = 0$ ):

$$\psi_M = \psi_H = 0. \quad (15)$$

(4) Unstable condition ( $Ri_B < 0$ ):

$$\psi_M = 2 \ln \frac{1+x}{2} + \ln \frac{1+x^2}{2} - 2 \arctan(x) + \frac{\pi}{2}, \quad (16a)$$

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

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

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

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

$$\theta_* = \frac{k(\theta - \theta_g)}{R \left[ \ln \frac{z}{z_{0h}} - \psi_H \right]}, \quad (18)$$

~~The calculation procedure of the Li scheme is the following: (1) determine  $Ri_B$ ,  $z_{0m}$  and  $z_{0h}$  according to the observation data; (2) calculate  $\zeta$  with  $Ri_B$ ,  $z_{0m}$  and  $z_{0h}$ ; (3) calculate the momentum and sensible heat fluxes under different conditions. The MM5 scheme is summarized as follows: (1) determine the universal functions according to the values of  $Ri_B$  and  $z_0$ ; (2) calculate the  $u_*$  and  $\theta_*$  with the meteorological variables and flux data; (3) derive the turbulent fluxes. Compared with other non-iterative schemes including MM5, the Li scheme can be applied to the full range of roughness status  $10 \leq \frac{z}{z_{0m}} \leq 10^5$  and  $-0.5 \leq \ln \frac{z_{0m}}{z_{0h}} \leq 30$  under whole conditions  $-5 \leq Ri_B \leq 2.5$ . 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 condition; (3) Li considers the RSL effect while MM5 ignores it. Overall, the universal functions in different conditions are determined by  $Ri_B$  and  $z_0$ . Then  $u_*$  and  $\theta_*$  will be calculated with meteorological data and flux data. At last, the turbulent fluxes are derived by Eqs. (1a) and (1b).~~

### 3 Observational data and methods

~~The observational fluxes used in this study measured at data was from Gucheng station from December 1, 2016 to January 9, 2017, (GC), which is in China Atmosphere Watch Network (CAWNET) and located in the southwest of Beijing about 110km, at 115.40 E, 39.08 N. In winter, the station surface was covered with wheat and the surrounding areas were mainly farmland and scattered villages (Fig. 1). The eddy correlation flux measurement system is mainly composed of a three dimensional (3D) Temperature measurement with a sonic anemometer (CSAT3) and a fast response infrared gas~~

239 analyzer (LI-7500) at 4m height. The data was collected from December 1, 2016 to January 9, 2017 including momentum  
240 fluxes, heat fluxes, wind speed and wind direction, air temperature, density of air and vapor, pressure with 30 minutes  
241 interval. Besides, there were radiation data provided by the net radiation sensor (CNR1) including the surface upward long  
242 wave radiation and the long wave radiation incident to the ground surface and PM<sub>2.5</sub> data provided by the Environmental  
243 Protection Station of China's Ministry of Environmental Protection (EPS/CMEP): Gucheng station (115.40° E, 39.08° N) is  
244 located at Gucheng County, Baoding, Hebei province and it is about 110km southwest of Beijing (Fig. 1a). This station has a  
245 farmland site where rice is planted in summer and wheat in winter. The surroundings are mainly farmland and scattered  
246 villages (Fig. 1b). At Gucheng station, the momentum and sensible heat fluxes near surface were measured by the eddy  
247 correlation flux measurement system. The system is mainly composed of a sonic anemometer (CSAT3) and a gas analyzer  
248 (LI-7500). They are set up at 4m height above surface ground. The measured fluxes are used to evaluate the two schemes as  
249 well as estimate the roughness lengths. The measured meteorological variables including wind speed and direction,  
250 temperature, humidity, pressure, radiation are used to calculate the momentum and sensible heat fluxes both in the Li and  
251 MM5 schemes. Note the observed meteorological data were from Gucheng station and national basic automatic weather  
252 stations in Jing-Jin-Ji in east China, respectively. Hourly surface PM<sub>2.5</sub> mass concentration in Baoding and Beijing from  
253 China National Environmental Monitoring Centre (<http://www.cnemc.cn/>) were also used in this paper.

### 254 3.1 Data processing

255 ~~In order to~~ To obtain accurate flux data, ~~it needs~~ quality control ~~has been performed for~~ the observational data,  
256 including: (1) eliminated the outliers and the data in rainy days; (2) double rotation and WPL correction (Webb et al., 1980);  
257 (3) omit the dataset when the wind speed are less than 0.5m/s, ~~as well as correcting momentum by using a double axis~~  
258 ~~rotation for the sonic anemometer tilt correction and correcting sensible heat fluxes by modifying sonic virtual temperature.~~  
259 In addition, ~~the wind field especially the wind direction has a great impact on the value of  $z_{0m}$ , so it is necessary to~~  
260 ~~understand the situation at Gucheng station, we considered the effect of wind field on the roughness length.~~ Fig. 2 shows ~~the~~  
261 distribution frequency of wind speed and wind direction at ~~GCGucheng~~ during ~~the~~ observations (December 1, 2016 ~  
262 January 9, 2017). The wind speed is stable during this period and the maximum is no more than 5 m/s and most of them are  
263 about 1 ~ 2 m/s. The wind direction is relatively uniform except for the southeast wind (135° ~~degrees~~). ~~Therefore, to avoid~~  
264 ~~the measurement error of the instrument, the wind speed data less than 0.5m/s are eliminated.~~

### 265 3.2 Determination of surface skin temperature

266 The surface skin temperature ~~at Gucheng station error caused by the CSAT3 is too large to be taken to calculate the flux~~  
267 ~~as input. Therefore, the surface skin temperature~~ is calculated from the radiation data ~~by the following formula: detected by~~  
268 ~~the CNR1 as:~~

269 
$$R_{lw}^{\uparrow} = (1 - \varepsilon_s)R_{lw}^{\downarrow} + \varepsilon_s \sigma T_g^4, \quad (19)$$

270 where  $R_{lw}^{\uparrow}$  and  $R_{lw}^{\downarrow}$  are the surface upward longwave radiation and long wave radiation incident on the surface,  
 271 respectively.  $\sigma$  is the Stephen Boltzmann constant,  $\sigma = 5.67 \times 10^{-8} \text{Wm}^{-2}\text{K}^{-4}$ .  $T_g$  is the surface skin temperature,  $\varepsilon_s$  is  
 272 the surface emissivity which is the prerequisite basis for calculating  $T_g$ . Many researches estimated  $\varepsilon_s$  and the range of the  
 273 values is always 0.9 ~ 1 (Stewart et al., 1994; Verhoef et al., 1997). According to the semi-empirical method in Yang et al.  
 274 (2008),  $\varepsilon_s$  is estimated when the RMSE is minimal. In this paper, the Li and MM5 schemes were used to estimate the  $\varepsilon_s$   
 275 value (as shown in Fig. 3). It is clear that the  $\varepsilon_s$  value corresponding to the minimum RMSE is not very sensitive to the  
 276 choice of two schemes. When  $\varepsilon_s$  is 1, the RMSE has the minimum value. Thus, this experiment we takes 1 as the optimal  
 277 value of  $\varepsilon_s$  to calculate  $T_g$  value.

278 **3.3 Determination of roughness length  $z_{0m}$  ( $z_{0h}$ )**

279 Using the observed momentum and sensible heat fluxes and the meteorological variables including wind speed,  
 280 temperature, humidity and pressure after quality control at Gucheng station,  $z_{0m}$  and  $z_{0h}$  were derived by Eqs. (20a) and  
 281 (20b) following Yang et al. (2003) and Sicart et al. (2014).

282 
$$\frac{u_*}{u} = \frac{k}{\ln \frac{z}{z_{0m}} - \psi_M} \quad (20a)$$

283 
$$\frac{\theta_*}{(\theta - \theta_g)} = \frac{k}{R[\ln \frac{z}{z_{0h}} - \psi_H]} \quad (20b)$$

284 During the observation period, the crops stopped growing and the height did not exceed 0.1 m, so the zero-plane  
 285 displacement height was ignored hence the reference height  $z$  was taken as 4m. The observation time was too short (about 1  
 286 month) to consider the effect of seasonal variations on roughness lengths. Thus,  $z_{0m}$  and  $z_{0h}$  were assumed as two fixed  
 287 values. Based on the variables and formulae mentioned above, the roughness lengths at Gucheng are derived:  $z_{0m} =$   
 288 0.0419 m,  $z_{0h} = 0.0042$  m.

289 **4 Results and discussion**

290 The RSL, roughness length and their influence on the calculation of turbulent flux are discussed in detail in this section.  
 291 The Li and MM5 schemes are offline tested and evaluated during the haze pollution from December 13 to 23, 2016. The  
 292 concept of roughness and its influence on the calculation of turbulent flux are going to be described in detail, and then the  
 293 value of  $z_{0m}$  and  $z_{0h}$  will be determined by theories above. Using  $z_{0m}$ ,  $z_{0h}$  and related observational data, we will have  
 294 offline tests on Li and MM5. Finally, the behavior of two schemes will be compared in a severe haze pollution at GC.



#### 295 4.1 The influence of roughness length on the calculation of turbulent flux

296 The RSL is usually defined as the region where the flow is influenced by the individual roughness elements as reflected  
297 by the spatial inhomogeneity of the mean flow (Florens et al., 2013). In the RSL, turbulence is strongly affected by  
298 individual roughness elements, and the standard MOST is no longer valid (Simpson et al., 1998). Therefore, it is necessary to  
299 consider the RSL effect in the calculation of turbulent fluxes, especially for the rough terrain such as forest or large cities.  
300  $z_{0m}$  is defined as the height at which the extrapolated wind speed following the similarity theory vanishes. It is mainly  
301 determined by land-cover type and canopy height after excluding large obstructions. In models,  $z_{0m}$  is always based on a  
302 look-up table which is related to land-cover types. In this paper study,  $z_{0m}$  is simply classified based on the research of Stull  
303 (1988) and is listed in Table 1. It can be seen in Table 1 that the rougher underlying surface corresponds to the larger value of  
304  $z_{0m}$ . more rough land surface is, the higher value of  $z_{0m}$  is. Thus, different land cover types have different effects on flux  
305 calculation.  $z_{0h}$  is the height at which the extrapolated air temperature is identical to the surface skin temperature, and it is  
306 also a scalar quantity. Some early researches assumed that  $z_{0m}$  was equal to  $z_{0h}$  (Louis, 1979; Louis et al., 1982).  
307 However, the assumption is not applicable in reality because  $z_{0m}$  and  $z_{0h}$  have different physical meanings. Different  
308 treatment of  $z_{0m}$  and  $z_{0h}$  may introduce considerable changes in the surface flux calculation (Launiainen, 1995; Kot and  
309 Song, 1998; Anurose and Subrahmanyam, 2013). Many studies removed the assumption that  $z_{0m}$  was equal to  $z_{0h}$  and  
310 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  
311 large (Wouters et al., 2012; Li et al., 2014; Li et al., 2015). Some field experiments even indicated the ratio  $z_{0m}/z_{0h}$  has a  
312 diurnal variation (Sun, 1999; Yang, 2003; Yang, 2008). In this study, we make the common assumption that the ratio  
313  $z_{0m}/z_{0h}$  is a constant. Thus, many following studies modified this assumption and made it more reliable in the situation that  
314  $z_{0m}$  was not equal to  $z_{0h}$  or the difference between two values was much large (e.g., Song, 1998; Wouters et al., 2012; Li  
315 et al., 2014; Li et al., 2015).

316 With the Li scheme, we test the effect of the roughness length on flux calculation. In the process, take  $z = 10\text{m}$  as the  
317 reference height and set the range of  $Ri_B$  according to Louis82 (Louis et al., 1982) from 2 to 1. Considering the lowest  
318 level in mesoscale models is usually about 10m,  $z = 10\text{ m}$  is set as the reference height. The range of  $Ri_B$  is set according  
319 to Louis82 (Louis et al., 1982) in the following discussion. Firstly, discuss the effect of  $z_{0m}$  on flux calculation. Set  
320  $\frac{z_{0m}}{z_{0h}} = 1$ , different land-cover types (different  $z_{0m}$  values) and RSL on flux calculation were discussed. Set  $z_{0m} = z_{0h}$ ,  
321 corresponding to four cases:  $z_{0m} = 1, 0.5, 0.05, 0.001\text{ m}$ . These cases correspond to large cities, forests, agricultural fields and  
322 wide water surface, respectively. Fig. 4 giveshows the relationship between  $C_M(C_H)$  and  $Ri_B$  for different  $z_{0m}$  values and  
323 treatment of RSL. It can be seen that both RSL and  $z_{0m}$  have impacts on  $C_M$  and  $C_H$ . Ignoring the RSL effect results in  
324 larger  $C_M$  and  $C_H$ , compared with the results of original scheme considering the RSL. The difference induced by RSL is  
325 obvious only under the rough surface. For example, the difference under  $z_{0m} = 1$  is obviously greater than other  $z_{0m}$

326 settings, and when  $z_{0m}$  is reduced to 0.05 or less, the RSL has little effect. Furthermore, the RSL contributes more to  
 327 sensible heat transfer than to momentum transfer under the same setting of  $z_{0m}$ . The effects of different land-cover types on  
 328  $C_M$  and  $C_H$  are much more significant compared with RSL. The effects of different land cover types on  $C_M$  and  $C_H$  are  
 329 significant under both the stable atmosphere ( $Ri_B > 0$ ) and the unstable atmosphere ( $Ri_B < 0$ ). The rougher the surface is  
 330 (corresponding to the larger  $z_{0m}$  value), the larger the  $C_M$  ( $C_H$ ) calculated momentum or sensible heat flux is. In addition,  
 331 there is a corresponding relationship between  $C_M$  ( $C_H$ ) and stability. The more unstable the atmosphere is, the larger  
 332 difference the value of  $C_M$  ( $C_H$ ) is and vice versa. Once the value of  $Ri_B$  exceeds the critical value (generally 0.2~0.25), the  
 333 transfer coefficients decline sharply but still above 0.

334 Secondly, the effects of difference between  $z_{0m}$  and  $z_{0h}$  as well as RSL on flux calculation are discussed. discuss the  
 335 effect of difference between  $z_{0m}$  and  $z_{0h}$  on flux calculation. The relationship between  $z_{0m}$  and  $z_{0h}$  can be expressed as  
 336  $kB^{-1} = \ln \frac{z_{0m}}{z_{0h}}$ . Over the sea,  $z_{0m}$  is comparable to  $z_{0h}$ ; over the uniform vegetation surface (e.g., grassland, farmland,  
 337 woodland),  $kB^{-1}$  is about 2 ( $z_{0m}/z_{0h} \approx 10$ ) (Garratt and Hicks, 1973; Garratt, 1978; Garratt and Francey, 1978), which  
 338 coincides with our results in Gucheng ( $z_{0m} = 0.0419$  m,  $z_{0h} = 0.0042$  m); over the surface with bluff roughness elements,  
 339 the  $\frac{z_{0m}}{z_{0h}}$  value may be very large. For example, in some large cities,  $kB^{-1}$  can reach 30 ( $z_{0m}/z_{0h} \approx 10^{13}$ ) (Sugawara and  
 340 Narita, 2009). Therefore, the ratio  $z_{0m}/z_{0h} \frac{z_{0m}}{z_{0h}}$  value can varies over a wide range. Fig. 5 shows the relationship between  
 341  $C_M$  ( $C_H$ ) and  $Ri_B$  for different treatment of  $z_{0m}/z_{0h} \frac{z_{0m}}{z_{0h}}$  values. Set  $z_{0m} = 1$  as a large city case,  $z_{0h} = 1, 0.01, 10^{-4}, 10^{-6}$  m,  
 342 and the large difference derived from the different ratios are displayed in Fig. 5. The similar RSL effect can be found  
 343 compared with Fig. 4. The differences induced by RSL are more obvious than that in Fig. 4. The different treatment of ratio  
 344  $z_{0m}/z_{0h}$  has great impact on turbulent flux transfer, particularly for sensible heat transfer. It seems evident that when  $z_{0h}$  is  
 345 not equal to  $z_{0m}$  ( $z_{0m}/z_{0h} = 100 \sim 10^6$ ), the calculated  $C_H$  is much small compared to the treatment that  $z_{0h}$  is equal to  
 346  $z_{0m}$  ( $z_{0m}/z_{0h} = 1$ ). In addition,  $C_M$  ( $C_H$ ) decreases with the increase of stability, and they decrease much slower when  $z_{0h}$   
 347 is not equal to  $z_{0m}$ . The larger the ratio is, the slower  $C_M$  ( $C_H$ ) falls with a rising stability. These results show that  
 348 distinguishing between  $z_{0m}$  and  $z_{0h}$  has great impact on flux calculation which is closely related to severe haze pollution.  
 349 Ignoring the difference between the two may lead to large errors in flux calculation and finally in air quality modeling.

#### 350 4.2 The determination of roughness length $z_{0m}$ ( $z_{0h}$ )

351 Based on above description and discussion, it can be seen that the determination of the appropriate value of  $z_{0m}$  ( $z_{0h}$ )  
 352 is a key and basis for calculation of surface turbulent fluxes. Using observational flux data with quality control,  $z_{0m}$  and  
 353  $z_{0h}$  are derived by Eq. (20a) and (20b) following Yang et al. (2003) and Sicart et al. (2014).

$$354 \frac{u_*}{u_*} = \frac{k}{\ln \frac{z}{z_{0m}} = 1/k} \quad (20a)$$

$$\frac{\theta_z}{(\theta - \theta_g)} = \frac{k}{R \left[ \ln \frac{z}{z_{0m}} - \psi_{H1} \right]} \quad (20b)$$

During the observation period, the crops stopped growing and the height did not exceed 0.1 m, so the zero plane displacement height can be ignored. The observation time is too short (about 1 month) to consider the effect of seasonal variations on roughness. Thus, assume  $z_{0m}$  and  $z_{0h}$  are two fixed values. Given the observational data, a dataset of  $z_{0m}$  ( $z_{0h}$ ) then is generated. Finally take median of the dataset as typical values of  $z_{0m}$  and  $z_{0h}$  for GC site:  $z_{0m} = 0.0419\text{m}$ ,  $z_{0h} = 0.0042\text{m}$ . These results are comparable to the typical values for agricultural fields ( $z_{0m} = 0.05$ ,  $z_{0m}/z_{0h} = 10$ ) discussed above. Therefore, the results are considered credible.

#### 4.3.2 Comparison of two schemes for calculating momentum and sensible heat fluxes calculated by the two schemes

Using the ~~calculated~~ obtained roughness lengths and the ~~relative~~ observations, the momentum and sensible heat flux were calculated by the 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  $z_{0m}$  in the MM5 scheme to calculate the momentum and sensible heat fluxes and they are going to be tested offline to compare their calculations of the momentum and sensible heat flux (Fig. 6). Firstly, take  $z_{0m} = 0.0419$  and  $z_{0h} = 0.0042$  in the Li scheme,  $z_0 = z_{0m} = 0.0419$  in the MM5 scheme to calculate the momentum and sensible heat fluxes and the comparison results are shown in Figs. 6a and 6b. It can be seen that ~~C~~ compared with MM5, Li performs better with higher regression coefficient and determination coefficient. For momentum fluxes, the regression coefficient ~~in~~ by Li is 0.6795 and that ~~in~~ by MM5 is 0.5598, indicating that the error of Li is 12% lower than that of MM5. For sensible heat fluxes, the regression coefficient ~~by~~ in Li is 0.7967 and that ~~in~~ by MM5 is 1.7994. The latter is much larger than 1, that is, which says the MM5 scheme obviously overestimate the sensible heat due to it does not distinguish  $z_{0h}$  from  $z_{0m}$ . ~~at~~ Then, make  $z_0$  equal to 0.0042 in the MM5 scheme to re-calculate the sensible heat fluxes as shown in Fig. 6c. It can be seen the result has a great improvement after modifying  $z_0$  value and the regression coefficient by MM5 is 0.7363, indicating that the error was reduced by 54% after considering the  $z_{0h}$  effect. The result indicates that  $z_{0h}$  plays a key role in both the SL scheme and the sensible heat flux (Chen and Zhang, 2009; Chen et al., 2011). That is due to no distinction of roughness length in the MM5 scheme. In order to compare the difference of two schemes without considering the effect of roughness length, take  $z_0 = z_{0h} = 0.0042$  in the MM5 scheme to calculate the sensible heat fluxes as Fig. 6c. Compared with Fig. 6b, there is a great improvement after modifying  $z_0$  value that the regression coefficient in MM5 becomes 0.7363, which is indicated that the error of calculated sensible heat flux by MM5 was reduced by 54% after discriminating  $z_{0h}$  from  $z_{0m}$ . However, the error ~~in~~ caused by Li is still 56% lower than that ~~in~~ by MM5. This illustrates that in addition to the effect of roughness lengths, the algorithm of Li scheme itself (~~including the selection of universal functions and the consideration of the RSL effect~~) is more reasonable than ~~thate of~~ ate of MM5 scheme.

#### 4.43 The specific performance of the two scheme in the severe haze pollution

There were two obvious pollution processes during this observation period and one occurred during December 13 to 23, 2016. Fig. 7 shows the variations of hourly observed time-series of  $PM_{2.5}$  concentration as well as the momentum fluxes and sensible heat fluxes calculated by Li and MM5 schemes at Gucheng station in this process both for calculation and observation in this pollution episode. For the research purpose significance, only the variation of above variables in the daytime (set from 8:00 a.m. to 20:00 p.m.) is taken into account. Note in MM5,  $z_0$  was 0.0419 when calculate momentum fluxes and it was 0.0042 when calculate sensible heat fluxes. All analysis data are processed as hourly average. It needs to note that in MM5, take 0.0419 of  $z_0$  when calculate momentum fluxes and take 0.0042 of  $z_0$  when calculate sensible heat fluxes. As shown in Fig. 7, on the whole, the calculated results of momentum and sensible heat fluxes for the two schemes are generally consistent with the trend of the observations data. Specifically, for the momentum fluxes (Fig. 7a), the results of two schemes have little difference when the values of observed momentum fluxes are large or at the peak when the observed momentum fluxes are large, the calculated results of the two schemes have little difference. When the observed momentum fluxes are small, the Li scheme results are close to or less than the observations, while the MM5 scheme results are always higher than observations because of the limit of  $u_* = 0.1$  in this scheme. For the sensible heat fluxes (Fig. 7b), MM5 results are always lower than observations while Li results are closer to observations especially when the observed values are small. Furthermore,

Fig. 7 also shows the diurnal variation of  $PM_{2.5}$  during this process. According to the evolution of  $PM_{2.5}$  concentration, this characteristics of fluxes and  $PM_{2.5}$  concentration, the haze process is then divided into three stages: the no pollution clear stage (stage 1: 13~14), the accumulation transition stage (stage 2: 16~18) and the maintenance stage (stage 3: 21~22). to discuss and evaluate the two schemes. As shown in Fig. 7, in the clear stage before the pollution occurs (stage 1), the atmospheric stratification is unstable,  $PM_{2.5}$  concentration is low and there is a strong flux transport in the SL, the corresponding observations of the momentum and sensible heat flux are relatively high and they vary greatly. the daily change of them is also great. In the accumulation transition stage (stage 2), the atmosphere is changing from unstable to stable corresponding with hazes formation, the momentum and sensible heat fluxes gradually decreases and the daily variation also decreases. In the maintenance stage (stage 3), the atmospheric stratification is very stable, and flux transport in 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 closer to the observations compared with MM5 results in all three stages.

Fig. 8 shows the probability distribution functions (PDF) of the difference of momentum fluxes (Figs. 8a, 8c, 8e, 8g) and sensible heat fluxes (Figs. 8b, 8d, 8f, 8h) calculated by using Li and MM5 schemes from the observations in different stages at Gucheng station. In the whole pollution process, for momentum fluxes (Fig. 8a), the PDF of the difference by Li tends to cluster in a narrower range centered by 0, and the probability within  $\pm 0.005N m^{-2}$  is 46.82%, while this value by

415 ~~MM5 falls to 23.02%, compared with MM5, the distribution of bias from the Li scheme tends to cluster in a narrower range~~  
416 ~~centered by 0, and the probability of Li bias within  $\pm 0.005\text{N m}^{-2}$  is 46.82%. The probability of MM5 bias within this range~~  
417 ~~fall to 23.02%. For sensible heat fluxes (Fig. 8b), the PDF of the difference by Li is also more concentrated around 0 than~~  
418 ~~that by MM5, the distribution of bias from Li is still more concentrated around 0 than it is from MM5. The probabilities of~~  
419 ~~bias by Li and MM5 bias within  $\pm 2.5\text{W m}^{-2}$  are 32.54% and 13.49%, respectively. In stage 1, for momentum fluxes (Fig. 8c),~~  
420 ~~the probability of Li bias within  $\pm 0.005\text{N m}^{-2}$  is 38.09%. The bias of MM5 mainly concentrates~~~~The probability distribution~~  
421 ~~of MM5 bias focus on area larger than 0, and its-the probability within  $\pm 0.005\text{N m}^{-2}$  is 14.29%. For sensible heat fluxes (Fig.~~  
422 ~~8d), the probability of Li bias within  $\pm 2.5\text{W m}^{-2}$  is 38.09%, the same as momentum fluxes. The bias of MM5 mainly~~  
423 ~~concentrates~~~~The probability distribution of MM5 bias focus on area~~ less than 0, and ~~its-the~~ probability within  $\pm 2.5\text{W m}^{-2}$  is  
424 9.52%. In stage 2, the differences between the two schemes ~~are~~is more obvious. The momentum and sensible heat fluxes bias  
425 ~~by from~~ Li is the most concentrated around 0 in all cases, while the distribution of ~~bias by~~ MM5 ~~bias~~ is similar to that in stage  
426 1. Specifically, for momentum fluxes (Fig. 8e), the probabilities of Li bias and MM5 bias within  $\pm 0.005\text{N m}^{-2}$  are 56.25%  
427 and 25.00%. For sensible heat fluxes (Fig. 8f), the probabilities of ~~bias by Li bias~~ and MM5 ~~bias~~ within  $\pm 2.5\text{W m}^{-2}$  are 40.62%  
428 and 6.25%. In stage 3, the difference between two schemes is small. For momentum fluxes (Fig. 8g), the probabilities of ~~bias~~  
429 ~~by Li bias~~ and MM5 ~~bias~~ within  $\pm 0.005\text{N m}^{-2}$  are 22.73% and 27.27%. For sensible heat fluxes (Fig. 8h), the probabilities of  
430 ~~bias by Li bias~~ and MM5 bias within  $\pm 2.5\text{W m}^{-2}$  are both 36.36%.

431 ~~Mean bias (MB), normalized mean bias (NMB), normalized mean error (NME) and root mean square error (RMES) of~~  
432 ~~Li and MM5 were calculated to test the two schemes. Four common evaluation metrics were used to further test the abilities~~  
433 ~~of the Li and MM5 schemes in calculating fluxes (Table 2). They are the mean bias (MB), normalized mean bias (NMB),~~  
434 ~~normalized mean error (NME) and root mean square error (RMES). Table 2 shows that the Li scheme generally~~  
435 ~~estimates~~gives a better estimate than the MM5 scheme. In ~~the~~ whole ~~haze~~ process, the ~~momentum fluxes calculated by Li~~  
436 ~~scheme is~~ underestimates ~~ed~~ the momentum fluxes by 3.63% relative to the observations, while the ~~results calculated by MM5~~  
437 ~~scheme is~~ overestimates ~~ed~~ by 34.03%. ~~The Li and MM5 schemes underestimate the sensible heat fluxes by 15.69% and~~  
438 ~~50.22%, respectively. The sensible heat fluxes calculated by Li and MM5 are both underestimated and the underestimations~~  
439 ~~are 15.69% and 50.22%. In the three selected stages, the Li scheme performs much better than the MM5 scheme in the stage~~  
440 ~~1 and stage 2, first two stages. Especially in stage 2, when atmospheric stratification transforms from unstable to stable~~  
441 ~~condition, the difference between the Li and MM5 schemes are particularly significant, that is, the atmosphere transforming~~  
442 ~~from unstable to stable stratification, the difference between the Li and MM5 schemes are particularly significant. Both t~~  
443 ~~Li and MM5 schemes have overestimates for the momentum fluxes and the values are by 7.68% and 45.56, respectively,~~  
444 ~~while Li and MM5 Two schemes have underestimates for the sensible heat fluxes and the values are by 33.84% and 76.88%.~~  
445 ~~The error of Li is much less than that of MM5. It can be seen the Li scheme calculation error is much smaller than the MM5~~

446 ~~scheme error. Considering the importance of atmospheric stratification in the generation and accumulation of PM<sub>2.5</sub> in stage 2,~~  
447 ~~Li scheme is expected to show better performance in online simulation of PM<sub>2.5</sub> than MM5. This stage plays an important~~  
448 ~~role in the generation and accumulation of pollutants. How to simulate the atmospheric state in a more reasonable way is~~  
449 ~~also a critical issue for air pollution modeling. Therefore, the superiority of the Li scheme in the air pollution process,~~  
450 ~~especially in this stage is of great reference value for improving the forecast of pollutant concentration in the current air~~  
451 ~~quality model. In stage 3, the difference between the two schemes is not obvious.~~

452 Based on the good behavior of the Li scheme in Gucheng, the same experiment was performed at Beijing station to  
453 discuss the effect of different land-cover types on flux calculation for two schemes. For Beijing station, the assumption  
454  $z_{0m} = 1\text{m}$ ,  $z_{0m}/z_{0h} = 10^6$  was made to represent the surface condition of megacity due to a lack in situ measurements of  
455 surface turbulent flux. As shown in Fig. 9, the evolution of PM<sub>2.5</sub> concentration at Beijing station was also divided into three  
456 stages (stage 1: 13~15; stage 2: 17~19; stage 3: 20~21) just like Gucheng in the discussion. Compare to Fig. 7, there is a  
457 significant increase in the difference of momentum and sensible heat fluxes between Li and MM5 in Fig. 9. To be specific,  
458 the momentum transfer in Beijing is obviously larger than that in Gucheng due to the great increase of the urban  
459 aerodynamic roughness length ( $z_{0m}$ ). In the meanwhile, the difference between Li and MM5 has a further expansion at  
460 Beijing station compared with Gucheng. The sensible heat transfer by Li scheme has great difference between clear days and  
461 pollution days, which is, the sensible heat transfer changes acutely in the stage 1 while it changes smoothly in the stage 2 and  
462 stage 3. The sensible heat transfer by the MM5 scheme is significantly different compared with Li result due to MM5  
463 ignored the  $z_{0m}$  effect, and the small number of  $z_{0h}$  keeps the sensible heat fluxes at a low level in all three stages.

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

$$465 \quad \Delta V = \left| \frac{V_{\text{Li}} - V_{\text{MM5}}}{V_{\text{MM5}}} \right| \times 100\%, \quad (21)$$

466 where  $V_{\text{Li}}$  and  $V_{\text{MM5}}$  are the momentum (or sensible heat) flux calculated by the Li and MM5 schemes, respectively. We  
467 obtained the relative differences at the two stations in the three stages through the statistics. It is clearly that the largest  
468 relative difference at Gucheng station is in the stage 2 and the value at Beijing station is in the stage 1. The differences in  
469 Beijing are always larger than that in Gucheng for each three stages. Specifically, the relative difference of momentum fluxes  
470 in stage 1, stage 2 and stage 3 increases by 73%, 34% and 27%, respectively, and the results of sensible heat fluxes are 289%,  
471 52% and 68%, respectively.

472 We further tested the two schemes in whole Jing-Jin-Ji region. Fig. 10 shows the mean momentum and sensible heat  
473 fluxes calculated by Li and MM5 schemes and their difference in Jing-Jin-Ji during the pollution episode. The assumption  
474  $z_{0m} = 0.1\text{m}$ ,  $z_{0m}/z_{0h} = 10^3$  were used to represent the average condition of the underlying surface of Jing-Jin-Ji region.  
475 As shown in Fig. 10, the momentum fluxes calculated by Li are less than that by MM5 in most stations; the sensible heat  
476 fluxes calculated by Li are usually larger than that by MM5. The result is consistent with the experiment of Gucheng station.

477 which further indicates the importance of considering  $z_{0m}$  and  $z_{0h}$  at the same time.

## 479 5 Conclusions

480 Using the observed momentum and sensible heat fluxes, together with conventional meteorological data including  
481 pressure, temperature, humidity and wind speed~~The applicability in describing the atmospheric stratification related with~~  
482 ~~severe haze in east China of the Li and MM5 schemes are evaluated and discussed. The observed momentum and sensible~~  
483 ~~heat fluxes, together with conventional meteorological data~~ from December 1, 2016 to January 9, 2017, including a severe  
484 pollution episode from December 13 to 23, 2016, the differences and the performance of the two surface schemes were  
485 discussed and evaluated in this paper. The evolution process of atmospheric stratification from unstable to stable  
486 corresponding to  $PM_{2.5}$  increasing was mainly discussed. The contributions of roughness lengths ( $z_{0m}$  and  $z_{0h}$ ) and other  
487 factors in the SL schemes to the momentum and sensible heat flux calculation were also discussed in details.~~are used to do~~  
488 ~~that. The transitional stage of atmospheric stratification from unstable to stable, corresponding to accumulation of  $PM_{2.5}$ , is~~  
489 ~~mainly discussed in this paper. The contributions of roughness lengths ( $z_{0m}$  and  $z_{0h}$ ) as well as the algorithms of the~~  
490 ~~momentum and sensible heat flux calculation are discussed. The results are summarized as follows:~~

491 1)  $z_{0m}$  and  $z_{0h}$  have important effects on turbulent flux calculation in the SL schemes. Different values of  $z_{0m}$  and  
492  $z_{0h}$  in the schemes could induce great changes in flux calculation, indicating that it is very necessary and important to  
493 distinguish  $z_{0h}$  from  $z_{0m}$ . Ignoring the  $z_{0h}$  effect in the MM5 scheme led to large errors in calculation of sensible  
494 heat fluxes and this error in Gucheng is 54%. Besides the roughness lengths, the algorithms of two schemes are also one  
495 of important factors. In addition, ignoring the effect of the RSL in schemes may also results in certain bias of  
496 momentum and sensible heat fluxes in megacity regions which represent the rough underlying surface.  $\frac{z_{0m}}{z_{0h}}$  and  $\frac{z_{0m}}{z_{0h}}$   
497 both reflect the condition of underlying surface and impact flux calculation greatly. Under the same condition, the larger  
498  $\frac{z_{0m}}{z_{0h}}$  (indicating rougher surface) is, the larger the calculated fluxes are. The fluxes over large cities ( $\frac{z_{0m}}{z_{0h}} = 1$ ) is quite  
499 different from those over agricultural fields ( $\frac{z_{0m}}{z_{0h}} = 0.05$ , similar to the value at GC). When  $\frac{z_{0m}}{z_{0h}}$  is larger, the value of  
500  $\frac{z_{0m}}{z_{0h}}$  should be larger, and the larger the value of  $\frac{z_{0m}}{z_{0h}}$  is, the greater the differences of calculated fluxes are. Especially,  
501 for a super city like Beijing, the value of  $\frac{z_{0m}}{z_{0h}}$  may be much larger than  $10^6$  and ignoring the difference between  $z_{0m}$   
502 and  $z_{0h}$  may lead to much uncertainties in flux calculation. It is very necessary to distinguish between  $z_{0m}$  and  $z_{0h}$  in  
503 SL scheme, which is probably beneficial to improve simulation of regional atmosphere stratification over urban  
504 agglomeration with rough surface and then  $PM_{2.5}$  during hazes.

505 2) The effect of  $z_{0m}/z_{0h}$  on turbulent fluxes is closely related to the land-cover types ( $z_{0m}$ ). A rough land-cover type  
506 (large  $z_{0m}$ ) should be accompanied by a large value of  $z_{0m}/z_{0h}$ . The differences of momentum and sensible heat fluxes  
507 calculated by Li and MM5 were much bigger in Beijing than that in Gucheng. This suggests that the MM5 scheme probably  
508 induces bigger error in megacities with rough surface (e.g., Beijing) than it in suburban area with smooth surface (e.g.,  
509 Gucheng) due to the irrational algorithm of MM5 scheme itself and the ignoring difference between  $z_{0m}$  and  $z_{0h}$ .

510 2) It could be seen from the regression coefficients and determination coefficients between calculated fluxes by the two  
511 schemes and observed fluxes of 40 days that the Li scheme was better than the MM5 scheme in general. For the  
512 momentum fluxes, the determination coefficients of Li and MM5 was about 0.41 and 0.40. Both schemes passed the  
513 significance level of 99.9%. The regression coefficient of Li was 0.68, and it generally reduced the error by 12%  
514 compared with MM5. When  $z_{0m}$  and  $z_{0h}$  took the same value ( $z_0 = z_{0m} = 0.0419$ ) in MM5, the sensible heat fluxes  
515 were obvious overestimated. When  $z_{0h}$  was taken into account ( $z_0 = z_{0h} = 0.0042$ ) in MM5, the calculated fluxes  
516 were significant improved and the error was reduced by 54%. However, this error was still higher about 5% compared  
517 with the Li scheme, illustrating that apart from the impact of roughness length, the different algorithms of the two  
518 schemes also achieves obvious differences in calculated fluxes.

519 3) The Li scheme generally performed better than the MM5 scheme in the calculation of both the momentum flux and  
520 the sensible heat flux compared with observations at Gucheng station. The Li scheme made a better description in  
521 atmospheric stratification which is closely related to the haze pollution, compared with the MM5 scheme. This advantage of  
522 Li scheme was the most prominent in the transition stage from unstable to stable atmospheric stratification corresponding to  
523 the  $PM_{2.5}$  accumulation. In this stage, the momentum flux calculated by Li was overestimated by 7.68% and this  
524 overestimation by MM5 was up to 45.56%; the sensible heat flux by Li was underestimated by 33.84% while this  
525 underestimation by MM5 was even up to 76.88%. In most Jing-Jin-Ji region, the momentum fluxes calculated by Li were  
526 less than that by MM5 and the sensible heat fluxes by Li were larger than that by MM5, which was consistent with Gucheng.

527 3) During the heavy pollution process, the calculated momentum and sensible heat fluxes by the Li scheme were better  
528 than those by the MM5 scheme generally. Especially in the  $PM_{2.5}$  accumulated stage, the advantages of Li were more  
529 prominent. Compared with MM5, the probability distributions of both the momentum and sensible heat flux bias of Li  
530 tended to cluster in a narrower range centered by 0. The calculated momentum fluxes by Li were overestimated by 7.68%  
531 and this overestimation by MM5 was up to 45.56%. The calculated sensible heat fluxes by Li were underestimated by  
532 33.84% while this underestimation by MM5 was even up to 76.88%.

533 The offline study in this paper showed that of two SL-Li schemes in this paper showed the superiority of the Li –was  
534 superior to the MM5 scheme for surface flux calculation corresponding to the  $PM_{2.5}$  evolution during the haze episode in  
535 Jing-Jin-Ji in east China in general. This superiority was even more remarkable during the atmosphere transforming stage



536 from unstable to stable stratification. However, the comparison of the two schemes focusing on more underlying surfaces  
537 (e.g., super cities and agricultural fields) could not be conducted at present due to the shortage of observed fluxes data, which  
538 should be discussed in detail in next paper when the sufficient data is available. The offline study results of this paper only  
539 offer prerequisite a basic and a possible way to improve PBL diffusion simulation and then PM<sub>2.5</sub> prediction, which will be  
540 achieved in the follow-up work of online integrating of the Li scheme into the atmosphere chemical model.

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#### 545 References

- 546 Ban, J.M., Gao, Z.Q., Lenschow, D. H., 2010. Climate simulations with a new air-sea turbulent flux parameterization in the  
547 National Center for Atmospheric Research Community Atmosphere Model (CAM3). *J. Geophys. Res.* 115.
- 548 Beljaars, A.C.M., Holtslag, A.A.M., 1991. Flux parameterization over land surfaces for atmospheric models. *J. Appl. Meteor.*  
549 30, 327-341.
- 550 Businger, J.A., 1966. Transfer of momentum and heat in the planetary boundary layer. in *Proceedings of a Symposium on*  
551 *Arctic Heat Budget and Atmospheric Circulation*. 305-331. The RAND Corp., Santa, Monica, Calif.
- 552 Businger, J.A., Wyngaard, J.C., Izumi, Y., Bradley, E. F., 1971. Flux profile relationships in the atmospheric surface layer.  
553 *J. Atmos. Sci.* 28, 181-189.
- 554 Cheng, Y., Brutsaert, W., 2005. Flux profile relationships for wind speed and temperature in the stable atmospheric  
555 boundary layer. *Bound. Layer Meteorol.* 114, 519-538.
- 556 Cheng, F.Y., Chin, S.C., Liu, T.H., 2012. The role of boundary layer schemes in meteorological and air quality simulations of  
557 the Taiwan area. *Atmos. Environ.* 54, 714-727.
- 558 Dyer, A.J., 1967. The turbulent transport of heat and water vapour in an unstable atmosphere. *Quart. J. Roy. Meteor. Soc.* 93,  
559 501-508.—
- 560 Dyer, A.J., 1974. A review of flux profile relationships. *Bound. Layer Meteorol.* 7, 363-372.—
- 561 Garratt, J.R., 1978. Transfer characteristics for a heterogeneous surface of large aerodynamic roughness. *Quart. J. Roy.*  
562 *Meteor. Soc.* 104, 491-502.—
- 563 Garratt, J.R., Hicks, B.B., 1973. Momentum, heat and water vapour transfer to and from natural and artificial surfaces. *Quart.*  
564 *J. Roy. Meteor. Soc.* 99, 680-687.

565 Garratt, J.R., Francey, R.J., 1978. Bulk characteristics of heat transfer in the unstable, baroclinic atmospheric boundary layer.  
566 Bound. Layer Meteorol. 15, 399-421. —

567 Högström, U., 1996. Review of some basic characteristics of the atmospheric surface layer. Bound. Layer Meteorol. 78,  
568 215-246.

569 Holtslag, A.A.M., de Bruin, H.A.R., 1988. Applied modeling of the nighttime surface energy balance over land. J. Appl.  
570 Meteor. 27, 689-704.

571 Hu, X.M., Nielsen-Gammon, J.W., Zhang, F.Q., 2010. Evaluation of three planetary boundary layer schemes in the WRF  
572 model. J. Appl. Meteorol. Climatol. 49, 1831-1844.

573 Jiménez, P.A., Dudhia, J., González-Rouco, J.F., Navarro, J., Montávez, J.P., García-Bustamante, E., 2012. A revised  
574 scheme for the WRF surface layer formulation. Mon. Wea. Rev. 140, 898-918.

575 Launiainen, J., 1995. Derivation of the relationship between the Obukhov stability parameter and the bulk Richardson  
576 number for flux-profile studies. Bound. Layer Meteorol. 76, 165-179. —

577 Li, Y.B., 2014. On the Surface Turbulent Fluxes Calculation in Numerical Models. Beijing: university of Chinese academy  
578 of sciences.

579 Li, Y., Gao, Z., Li, D., Wang, L., Wang, H., 2014. An improved non-iterative surface layer flux scheme for atmospheric  
580 stable stratification conditions. Geosci. Model Dev. 7, 515-529. —

581 Li, Y., Gao, Z., Li, D., Chen, F., Yang, Y., Sun, L., 2015. An Update of Non-iterative Solutions for Surface Fluxes Under  
582 Unstable Conditions. Bound. Layer Meteorol. 156, 501-511. —

583 Li, Y., Gao, Z., Li, D., Chen, F., Yang, Y., Sun, L., 2016. Erratum to: An Update of Non-iterative Solutions for Surface Fluxes  
584 Under Unstable Conditions. Bound. Layer Meteorol. 161: 225-228.

585 Louis, J. F., 1979. A parametric model of vertical eddy fluxes in the atmosphere. Bound. Layer Meteorol. 17, 187-202. —

586 Louis, J. F., Tiedtke, M., Geleyn, J. F., 1982. A short history of the operational PBL parameterization at ECMWF [C]// Proc.  
587 Workshop on Planetary Boundary Layer Parameterization. Shinfield Park, Reading, Berkshire, UK, European Centre  
588 for Medium Range Weather Forecasts. 59-79.

589 Monin, A., Obukhov, A., 1954. Osnovnye zakonomernosti turbulentnogo peremesivaniia v prizemnon sloe atmosfery (Basic  
590 laws of turbulent mixing in the atmosphere near the ground). Trudy geofiz. inst. AN SSSR. 24, 163-187.

591 Paulson, C. A., 1970. The mathematical representation of wind speed and temperature profiles in the unstable atmospheric  
592 surface layer. J. Appl. Meteorol. 9, 857-861.

593 Ridder, K.D., 2010. "Bulk Transfer Relations for the Roughness Sublayer." Bound. Layer Meteorol. 134, 257-267.

594 Sharan, M., Srivastava, P., 2014. A Semi-Analytical Approach for Parametrization of the Obukhov Stability Parameter in the  
595 Unstable Atmospheric Surface Layer. Bound. Layer Meteorol. 153, 339-353.

596 Sicart, J.E., Litt, M., Helgason, W., Tahar, V.B., Chaperon, T., 2014. A study of the atmospheric surface layer and roughness  
597 lengths on the high altitude tropical Zongo glacier, Bolivia. *J. Geophys. Res.* 119, 3793–3808.

598 Simpson, J.J., Thurtell, G.W., Neumann, H.H., Den Hartog, G., Edwards, G.C., 1998. The Validity of Similarity Theory in  
599 the Roughness Sublayer Above Forests. *Bound. Layer Meteorol.* 87, 69–99.

600 Song, Y., 1998. An Improvement of the Louis Scheme for the Surface Layer in an Atmospheric Modelling System.  
601 *Bound. Layer Meteorol.* 88, 239–254.

602 Stewart, J. B., Kustas, W. P., Humes, K. S., Nichols, W. D., Moran, M. S., de Bruin, H. A. R., 1994. Sensible Heat  
603 Flux Radiometric Surface Temperature Relationship for Eight Semiarid Areas. *J. Appl. Meteorol.* 33, 1110–1117.

604 Stull, R. B., 1988. *An Introduction to Boundary Layer Meteorology*, Kluwer Academic Publishers, Dordrecht.

605 Sugawara, H., Narita, K., 2009. Roughness length for heat over an urban canopy. *Theor. Appl. Climatol.* 95, 291–299.

606 Tymvios, F., Charalambous, D., Michaelides, S., Lelieveld, J., 2017. Interecomparison of boundary layer parameterizations  
607 for summer conditions in the eastern Mediterranean island of Cyprus using the WRF-ARW model. *Atmos. Res.* DOI:  
608 10.1016/j.atmosres.2017.09.011.

609 Verhoef, A., de Bruin, H. A. R., van den Hurk, B. J. J. M., 1997. Some Practical Notes on the Parameter  $kB1$  for Sparse  
610 Vegetation. *J. Appl. Meteorol.* 36, 560–572.

611 Wang, S., Wang, Q., Doyle, J., 2002. Some improvement of Louis surface flux parameterization. Preprints, 15th Symp. on  
612 Boundary Layers and Turbulence, Wageningen, Netherlands, *Amer. Meteor. Soc.*, 547–550.

613 Wang, H., Xue, M., Zhang, X. Y., Liu, H. L., Zhou, C. H., Tan, S. C., Che, H. Z., Chen, B., Li, T., 2015a. Mesoscale  
614 modeling study of the interactions between aerosols and PBL meteorology during a haze episode in Jing Jin Ji (China)  
615 and its nearby surrounding region—Part 1: Aerosol distributions and meteorological features. *Atmos. Chem. Phys.*  
616 15, 3257–3275.

617 Wang, H., Shi, G. Y., Zhang, X. Y., Gong, S. L., Tan, S. C., Chen, B., Che, H. Z., Li, T., 2015b. Mesoscale modeling study of  
618 the interactions between aerosols and PBL meteorology during a haze episode in China Jing Jin Ji and its near  
619 surrounding region—Part 2: Aerosols' radiative feedback effects. *Atmos. Chem. Phys.* 15, 3277–3287.

620 Webb, E. K., 1970. Profile relationships: The log-linear range, and extension to strong stability. *Quart. J. Roy. Meteor. Soc.*  
621 96, 67–90.

622 Wouters, H., De Ridder, K., van Lipzig, N. P. M., 2012. Comprehensive Parametrization of Surface Layer Transfer  
623 Coefficients for Use in Atmospheric Numerical Models. *Bound. Layer Meteorol.* 145, 539–550.

624 Xie, B., Fung, J. C. H., Chan, A., Lau, A., 2012. Evaluation of nonlocal and local planetary boundary layer schemes in the  
625 WRF model. *J. Geophys. Res.* 117(D12), 48–50.

626 Yang, K., Tamai, N., Koike, T., 2001. Analytical Solution of Surface Layer Similarity Equations. *J. Appl. Meteorol.* 40,

627 [1647-1653.](#)

628 [Yang, K., Koike, T., Yang, D., 2003. Surface Flux Parameterization in the Tibetan Plateau. Bound. Layer Meteorol. 106,](#)

629 [245-262.](#)

630 [Yang, K., Koike, T., Ishikawa, H., Kim, J., Li, X., Liu, H. Z., Liu, S. M., Ma, X. M., Wang, J. M., 2008. Turbulent Flux](#)

631 [Transfer over Bare Soil Surfaces: Characteristics and Parameterization. J. Appl. Meteorol. CLIM. 47, 276-290.](#)

632 [Zhang, D., Anthes, R. A., 1982. A high resolution model of the planetary boundary layer—Sensitivity tests and comparisons](#)

633 [with SESAME 79 data. J. Appl. Meteorol. 21, 1594-1609.](#)

634 [Anurose, T. J., and Subrahmanyam, D. B.: Improvements in Sensible Heat-Flux Parametrization in the High-Resolution](#)

635 [Regional Model \(HRM\) Through the Modified Treatment of the Roughness Length for Heat, Bound.-Lay. Meteorol.,](#)

636 [147, 569-578, <https://doi.org/10.1007/s10546-013-9799-9>, 2013.](#)

637 [Ban, J., Gao, Z., and Lenschow, D. H.: Climate simulations with a new air-sea turbulent flux parameterization in the](#)

638 [National Center for Atmospheric Research Community Atmosphere Model \(CAM3\), J. Geophys. Res.-Atmos., 115,](#)

639 [https://doi.org/10.1029/2009JD012802, 2010.](#)

640 [Beljaars, A. C. M., and Holtslag, A. A. M.: Flux parameterization over land surfaces for atmospheric models, J. Appl.](#)

641 [Meteor., 30, 327-341, 1991.](#)

642 [Businger, J. A., Wyngaard, J. C., Izumi, Y., and Bradley, E. F.: Flux-profile relationships in the atmospheric surface layer, J.](#)

643 [Atmos. Sci., 28, 181-189, 1971.](#)

644 [Businger, J. A.: Transfer of momentum and heat in the planetary boundary layer, Proc. Symp. Arctic Heat Budget and](#)

645 [Atmospheric Circulation, RM-5233-NSF, 305-331, 1966.](#)

646 [Chen, F., and Zhang, Y.: On the coupling strength between the land surface and the atmosphere: From viewpoint of surface](#)

647 [exchange coefficients, Geophys. Res. Lett., 36, <https://doi.org/10.1029/2009GL037980>, 2009.](#)

648 [Chen, Y., Yang, K., He, J., Qin, J., Shi, J., Du, J., and He, Q.: Improving land surface temperature modeling for dry land of](#)

649 [China, J. Geophys. Res.-Atmos., 116, <https://doi.org/10.1029/2011JD015921>, 2011.](#)

650 [Cheng, F. Y., Chin, S. C., and Liu, T. H.: The role of boundary layer schemes in meteorological and air quality simulations of](#)

651 [the Taiwan area, Atmos. Environ., 54, 714-727, <https://doi.org/10.1016/j.atmosenv.2012.01.029>, 2012.](#)

652 [Cheng, Y., and Brutsaert, W.: Flux-profile relationships for wind speed and temperature in the stable atmospheric boundary](#)

653 [layer, Bound.-Lay. Meteorol., 114, 519-538, <https://doi.org/10.1007/s10546-004-1425-4>, 2005.](#)

654 [De Ridder, K.: Bulk Transfer Relations for the Roughness Sublayer, Bound.-Lay. Meteorol., 134, 257-267,](#)

655 [https://doi.org/10.1007/s10546-009-9450-y, 2010.](#)

656 [Dyer, A. J.: A review of flux-profile relationships, Bound.-Lay. Meteorol., 7, 363-372, <https://doi.org/10.1007/BF00240838>,](#)

657 [1974.](#)

658 [Dyer, A. J.: The turbulent transport of heat and water vapour in an unstable atmosphere, \*Quart. J. Roy. Meteor. Soc.\*, 93,](#)  
659 [501-508, <https://doi.org/10.1002/qj.49709339809>, 1967.](#)

660 [Florens, E., Eiff, O., and Moulin, F.: Defining the roughness sublayer and its turbulence statistics, \*Exp. Fluids\*, 54, 1500,](#)  
661 [https://doi.org/10.1007/s00348-013-1500-z, 2013.](#)

662 [Garratt, J. R., and Francey, R. J.: Bulk characteristics of heat transfer in the unstable, baroclinic atmospheric boundary layer,](#)  
663 [Bound.-Lay. Meteorol., 15, 399-421, <https://doi.org/10.1007/BF00120603>, 1978.](#)

664 [Garratt, J. R., and Hicks, B. B.: Momentum, heat and water vapour transfer to and from natural and artificial surfaces, \*Quart.\*](#)  
665 [J. Roy. Meteor. Soc.](#), 99, 680-687, 1973.

666 [Garratt, J. R.: Transfer characteristics for a heterogeneous surface of large aerodynamic roughness, \*Quart. J. Roy. Meteor.\*](#)  
667 [Soc.](#), 104, 491-502, 1978.

668 [Högström, U.: Review of some basic characteristics of the atmospheric surface layer, \*Bound.-Lay. Meteorol.\*, 78, 215-246,](#)  
669 [https://doi.org/10.1007/BF00120937, 1996.](#)

670 [Holtlag, A. A. M., and De Bruin, H. A. R.: Applied modeling of the nighttime surface energy balance over land, \*J. Appl.\*](#)  
671 [Meteor.](#), 27, 689-704, 1988.

672 [Hu, X. M., Nielsen-Gammon, J. W., and Zhang, F.: Evaluation of three planetary boundary layer schemes in the WRF model,](#)  
673 [J. Appl. Meteorol. Climatol.](#), 49, 1831-1844, <https://doi.org/10.1175/2010JAMC2432.1>, 2010.

674 [Jiménez, P. A., Dudhia, J., González-Rouco, J. F., Navarro, J., Montávez, J. P., and García-Bustamante, E.: A revised scheme](#)  
675 [for the WRF surface layer formulation, \*Mon. Wea. Rev.\*, 140, 898-918, <https://doi.org/10.1175/MWR-D-11-00056.1>,](#)  
676 [2012.](#)

677 [Kot, S. C., and Song, Y.: An Improvement of the Louis Scheme for the Surface Layer in an Atmospheric Modelling System,](#)  
678 [Bound.-Lay. Meteorol.](#), 88, 239-254, <https://doi.org/10.1023/A:1001119329423>, 1998.

679 [Launiainen, J.: Derivation of the relationship between the Obukhov stability parameter and the bulk Richardson number for](#)  
680 [flux-profile studie, \*Bound.-Lay. Meteorol.\*, 76, 165-179, <https://doi.org/10.1007/BF00710895>, 1995.](#)

681 [Li, T., Wang, H., Zhao, T., Xue, M., Wang, Y., Che, H., and Jiang, C.: The Impacts of Different PBL Schemes on the](#)  
682 [Simulation of PM<sub>2.5</sub> during Severe Haze Episodes in the Jing-Jin-Ji Region and Its Surroundings in China, \*Adv.\*](#)  
683 [Meteorol.](#), <http://dx.doi.org/10.1155/2016/6295878>, 2016a.

684 [Li, Y., Gao, Z., Li, D., Chen, F., Yang, Y., and Sun, L.: An Update of Non-iterative Solutions for Surface Fluxes Under](#)  
685 [Unstable Conditions, \*Bound.-lay. Meteorol.\*, 156, 501-511, <https://doi.org/10.1007/s10546-015-0032-x>, 2015.](#)

686 [Li, Y., Gao, Z., Li, D., Chen, F., Yang, Y., and Sun, L.: Erratum to: An Update of Non-iterative Solutions for Surface Fluxes](#)  
687 [Under Unstable Conditions, \*Bound.-Lay. Meteorol.\*, 161: 225-228, 2016b.](#)

688 [Li, Y., Gao, Z., Li, D., Wang, L., and Wang, H.: An improved non-iterative surface layer flux scheme for atmospheric stable](#)  
689 [stratification conditions, \*Geosci. Model Dev.\*, 7, 515-529, <https://doi.org/10.5194/gmd-7-515-2014>, 2014.](#)

690 [Li, Y.: \*On the Surface Turbulent Fluxes Calculation in Numerical Models\*, Beijing: university of Chinese academy of](#)  
691 [sciences, 2014.](#)

692 [Li, Z., Guo, J., Ding, A., Liao, H., Liu, J., Sun, Y., Wang, T., Xue, H., Zhang, H., and Zhu, B.: Aerosol and boundary-layer](#)  
693 [interactions and impact on air quality, \*Natl. Sci. Rev.\*, 4, 810–833, <https://doi.org/10.1093/nsr/nwx117>, 2017.](#)

694 [Liu, T. T., Gong, S. L., He, J. J., Yu, M., Wang, Q. F., Li, H. R., Liu, W., Zhang, J., Li, L., Wang, X. G., Li, S. L., Lu, Y. L.,](#)  
695 [Du, H. T., Wang, Y. Q., Zhou, C. H., Liu, H. L. and Zhao, Q. C.: Attributions of meteorological and emission factors to](#)  
696 [the 2015 winter severe haze pollution episodes in China's Jing-Jin-Ji area, \*Atmos. Chem. Phys.\*, 17, 2971–2980,](#)  
697 [https://doi.org/10.5194/acp-17-2971-2017, 2017.](#)

698 [Louis, J. F.: A parametric model of vertical eddy fluxes in the atmosphere. \*Bound.-Lay. Meteorol.\*, 17, 187-202,](#)  
699 [https://doi.org/10.1007/BF00117978, 1979.](#)

700 [Louis, J. F., Tiedtke, M., and Geleyn, J. F.: A short history of the operational PBL parameterization at ECMWF, in \*Workshop\*](#)  
701 [on Planetary Boundary Layer Parameterization, November 1981, ECMWF, Reading, U.K., pp. 59–79, 1982.](#)

702 [Monin, A. S., and Obukhov, A. M.: Basic laws of turbulent mixing in the surface layer of the atmosphere, \*Contrib. Geophys.\*](#)  
703 [Inst. Acad. Sci., USSR, 24, 163–187, 1954.](#)

704 [Paulson, C. A.: The mathematical representation of wind speed and temperature profiles in the unstable atmospheric surface](#)  
705 [layer, \*J. Appl. Meteorol.\*, 9, 857-861, 1970.](#)

706 [Sharan, M., and Srivastava, P.: A Semi-Analytical Approach for Parametrization of the Obukhov Stability Parameter in the](#)  
707 [Unstable Atmospheric Surface Layer, \*Bound.-Lay. Meteorol.\*, 153, 339-353, <https://doi.org/10.1007/s10546-014-9948-9>,](#)  
708 [2014.](#)

709 [Sicart, J. E., Litt, M., Helgason, W., Tahar, V. B., and Chaperon, T.: A study of the atmospheric surface layer and roughness](#)  
710 [lengths on the high-altitude tropical Zongo glacier, Bolivia, \*J. Geophys. Res.-Atmos.\*, 119, 3793–3808,](#)  
711 [https://doi.org/10.1002/2013JD020615, 2014.](#)

712 [Simpson, I. J., Thurtell, G. W., Neumann, H. H., Den Hartog, G., and Edwards, G. C.: The Validity of Similarity Theory in](#)  
713 [the Roughness Sublayer Above Forests, \*Bound.-Lay. Meteorol.\*, 87, 69-99, <https://doi.org/10.1023/A:1000809902980>,](#)  
714 [1998.](#)

715 [Stewart, J. B., Kustas, W. P., Humes, K. S., Nichols, W. D., Moran, M. S., and De Bruin, H. A. R.: Sensible heat](#)  
716 [flux-radiometric surface temperature relationship for eight semiarid areas, \*J. Appl. Meteorol.\*, 33, 1110-1117, 1994.](#)

717 [Stull, R. B.: \*An Introduction to Boundary Layer Meteorology\*, Kluwer Academic Publishers, London, 1988.](#)

718 [Sugawara, H., and Narita, K.: Roughness length for heat over an urban canopy, Theor. Appl. Climatol., 95, 291-299,](#)  
719 <https://doi.org/10.1007/s00704-008-0007-7>, 2009.

720 [Sun, J.: Diurnal Variations of Thermal Roughness Height over a Grassland, Bound.-Lay. Meteorol., 92, 407-427,](#)  
721 <https://doi.org/10.1023/A:1002071421362>, 1999.

722 [Tymvios, F., Charalambous, D., Michaelides, S., and Lelieveld, J.: Intercomparison of boundary layer parameterizations for](#)  
723 [summer conditions in the eastern Mediterranean island of Cyprus using the WRF-ARW model, Atmos. Res., 208, 45-59,](#)  
724 <https://doi.org/10.1016/j.atmosres.2017.09.011>, 2017.

725 [Vautard, R., Moran, M. D., Solazzo, E., Gilliam, R. C., Matthias, V., Bianconi, R., Chemel, C., Ferreira, J., Geyer, B.,](#)  
726 [Hansen, A. B., Jericevic, A., Prank, M., Segers, A., Silver, J. D., Werhahn, J., Eolke, R., Rao, S. T., and Galmarini, S.:](#)  
727 [Evaluation of the meteorological forcing used for the Air Quality Model Evaluation International Initiative \(AQMEII\)](#)  
728 [air quality simulations, Atmos. Environ., 53, 15-37, https://doi.org/10.1016/j.atmosenv.2011.10.065](#), 2012.

729 [Verhoef, A., De Bruin, H. A. R., and Van Den Hurk, B. J. J. M.: Some Practical Notes on the Parameter kB-1 for Sparse](#)  
730 [Vegetation., J. Appl. Meteorol., 36, 560-572, 1997.](#)

731 [Wang, H., Shi, G. Y., Zhang, X. Y., Gong, S. L., Tan, S. C., Chen, B., Che, H. Z., and Li, T.: Mesoscale modeling study of the](#)  
732 [interactions between aerosols and PBL meteorology during a haze episode in China Jing-Jin-Ji and its near surrounding](#)  
733 [region - Part 2: Aerosols' radiative feedback effects, Atmos. Chem. Phys., 15, 3277-3287,](#)  
734 <https://doi.org/10.5194/acp-15-3277-2015>, 2015b.

735 [Wang, H., Tan, S. C., Wang, Y., Jiang, C., Shi, G., Zhang, M., and Che, H. Z.: A multisource observation study of the severe](#)  
736 [prolonged regional haze episode over eastern China in January 2013, Atmos. Environ., 89, 807-815,](#)  
737 <https://doi.org/10.1016/j.atmosenv.2014.03.004>, 2014.

738 [Wang, H., Xue, M., Zhang, X. Y., Liu, H. L., Zhou, C. H., Tan, S. C., Che, H. Z., Chen, B., and Li, T.: Mesoscale modeling](#)  
739 [study of the interactions between aerosols and PBL meteorology during a haze episode in China Jing-Jin-Ji and its](#)  
740 [nearby surrounding region - Part 1: Aerosol distributions and meteorological features, Atmos. Chem. Phys., 15,](#)  
741 [3257-3275, https://doi.org/10.5194/acp-15-3257-2015](https://doi.org/10.5194/acp-15-3257-2015), 2015a.

742 [Wang, S., Wang, Q., and Doyle, J.: Some improvements to Louis surface flux parameterization. Paper presented at 15th](#)  
743 [symposium on boundary layers and turbulence, American Meteorological Society, 15-19 July 2002, Wageningen,](#)  
744 [Netherlands.](#)

745 [Webb, E. K., Pearman, G. I., and Leuning, R.: Correction of flux measurements for density effects due to heat and water](#)  
746 [vapour transfer, Quart. J. Roy. Meteor. Soc., 106, 85-100, 1980.](#)

747 [Webb, E. K.: Profile relationships: The log-linear range, and extension to strong stability, Quart. J. Roy. Meteor. Soc., 96,](#)  
748 [67-90, 1970.](#)

749 [Wouters, H., De Ridder, K., and van Lipzig, N. P. M.: Comprehensive Parametrization of Surface-Layer Transfer](#)  
750 [Coefficients for Use in Atmospheric Numerical Models, Bound.-Lay. Meteorol., 145, 539-550,](#)  
751 <https://doi.org/10.1007/s10546-012-9744-3>, 2012.

752 [Xie, B., Fung, J. C. H., Chan, A., and Lau, A.: Evaluation of nonlocal and local planetary boundary layer schemes in the](#)  
753 [WRF model, J. Geophys. Res.- Atmos., 117, 48-50, https://doi.org/10.1029/2011JD017080](#), 2012.

754 [Yang, K., Koike, T., and Yang, D.: Surface Flux Parameterization in the Tibetan Plateau, Bound.-Lay. Meteorol., 106,](#)  
755 <https://doi.org/10.1023/A:1021152407334>, 2003.

756 [Yang, K., Koike, T., Ishikawa, H., Kim, J., Li, X., Liu, H., Liu, S., Ma, Y., and Wang, J.: Turbulent Flux Transfer over](#)  
757 [Bare-Soil Surfaces: Characteristics and Parameterization, J. Appl. Meteorol. Clim., 47, 276-290,](#)  
758 <https://doi.org/10.1175/2007jame1547.1>, 2008.

759 [Yang, K., Tamai, N., and Koike, T.: Analytical Solution of Surface Layer Similarity Equations, J. Appl. Meteorol., 40,](#)  
760 [1647-1653, 2001.](#)

761 [Yang, Y., Liu, X., Qu, Y., Wang, J., An, J., Zhang, Y., and Zhang, F.: Formation mechanism of continuous extreme haze](#)  
762 [episodes in the megacity Beijing, China, in January 2013, Atmos. Res., 155, 192-203,](#)  
763 <https://doi.org/10.1016/j.atmosres.2014.11.023>, 2015.

764 [Zhang, B., Wang, Y., and Hao, J.: Simulating aerosol-radiationcloud feedbacks on meteorology and air quality over eastern](#)  
765 [China under severe haze conditions in winter, Atmos. Chem. Phys., 15, 2387-2404,](#)  
766 <http://doi.org/10.5194/acp-15-2387-2015>, 2015.

767 [Zhang, D., and Anthes, R. A.: A high-resolution model of the planetary boundary layer—Sensitivity tests and comparisons](#)  
768 [with SESAME-79 data, J. Appl. Meteorol., 21, 1594-1609, 1982.](#)

769 [Zhang, R., Li, Q., and Zhang, R.: Meteorological conditions for the persistent severe fog and haze event over eastern China](#)  
770 [in January 2013, Sci. China Earth Sci., 57, 26-35, https://doi.org/10.1007/s11430-013-4774-3](#), 2014.

771 [Zhong, J., Zhang, X., Dong, Y., Wang, Y., Liu, C., Wang, J., Zhang, Y., and Che, H.: Feedback effects of boundary-layer](#)  
772 [meteorological factors on cumulative explosive growth of PM<sub>2.5</sub> during winter heavy pollution episodes in Beijing](#)  
773 [from 2013 to 2016, Atmos. Chem. Phys., 18, 247-258, https://doi.org/10.5194/acp-18-247-2018](#), 2018.

774



775 **Table 1.** Typical values of  $z_{0m}$  corresponding to various land-cover types

$z_{0m}/m$	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
$10^{-4}$ ~ $10^{-3}$	The snow surface, wide water surface, flat deserts
$10^{-5}$	The ice surface

776

777

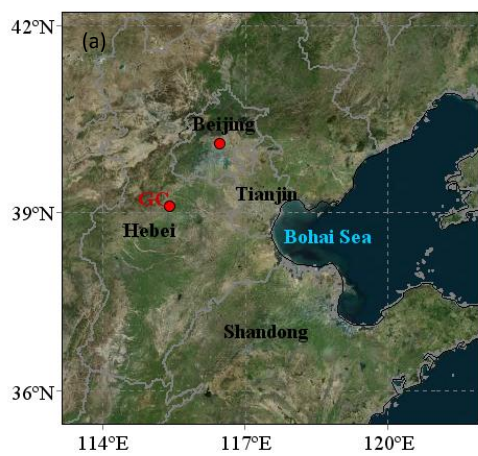
778

779 **Table 2.** Statistics between the Li and MM5 schemes calculated turbulent flux.

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

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

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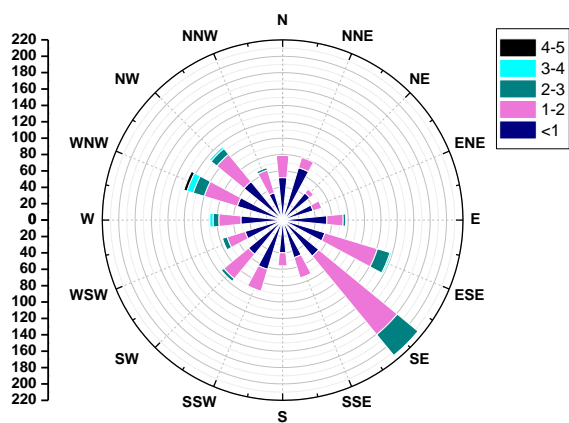
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784 | **Figure 1.** Location (a) and geographical environment (b) at [GCGucheng station](#). The map is from Bing Maps.

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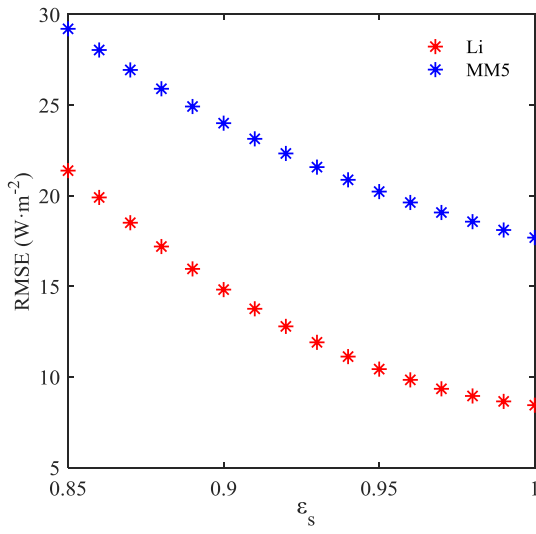
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789 | **Figure 2.** Wind Rose map at [GCGucheng station](#) from December 1, 2016, to January 9, 2017.

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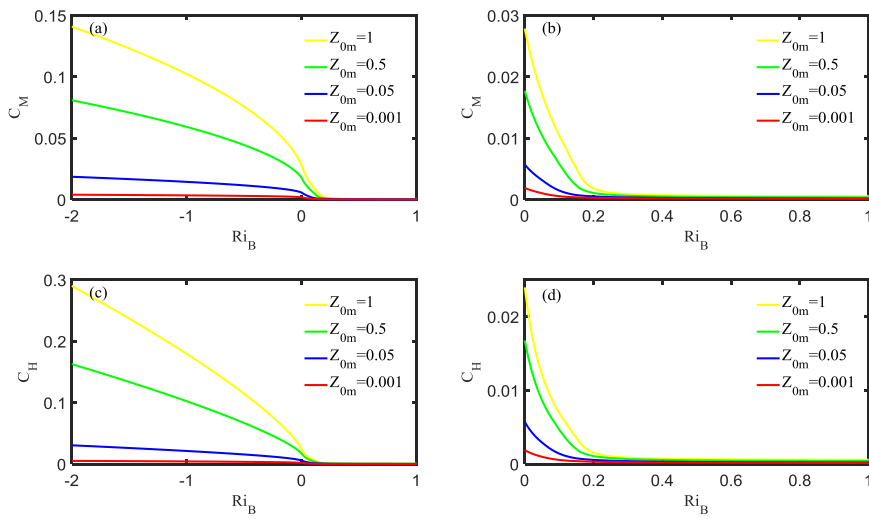
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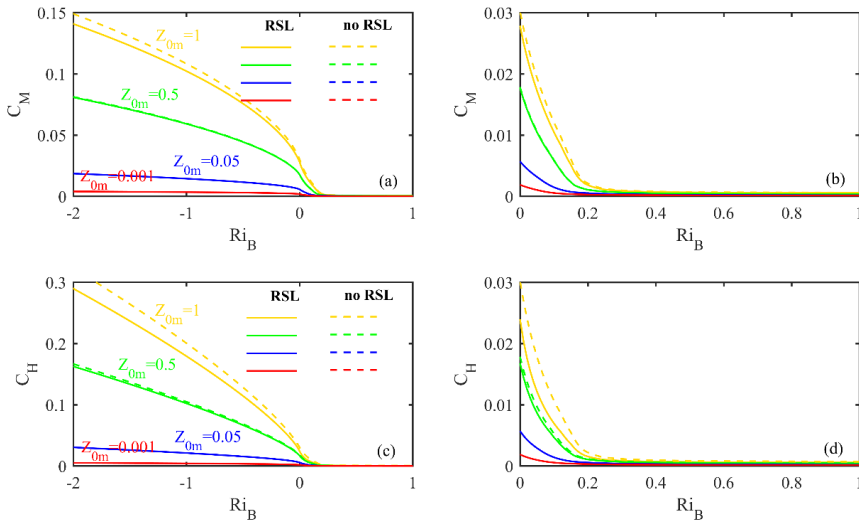
**Figure 3.** The surface emissivity  $\varepsilon_s$  dependence of RMSE between observed near-neutral heat fluxes and parameterized heat fluxes (red for Li and blue for MM5) at [GCGucheng station](#).



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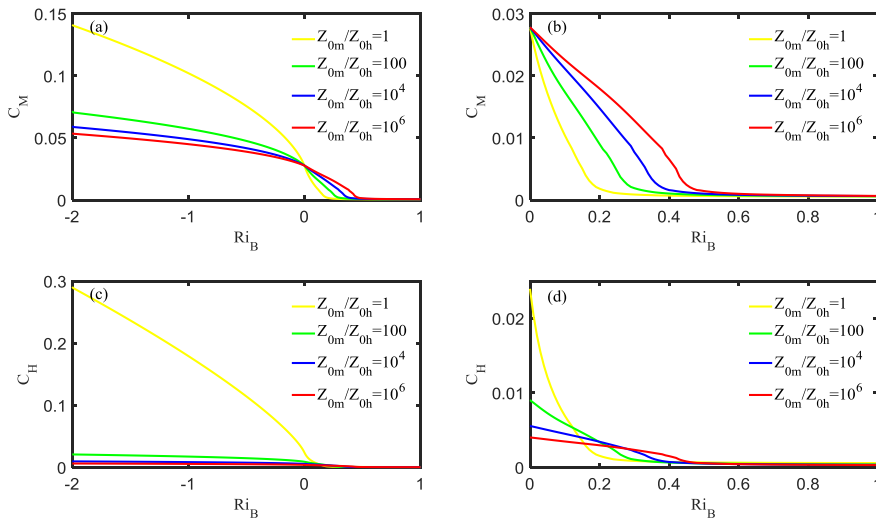
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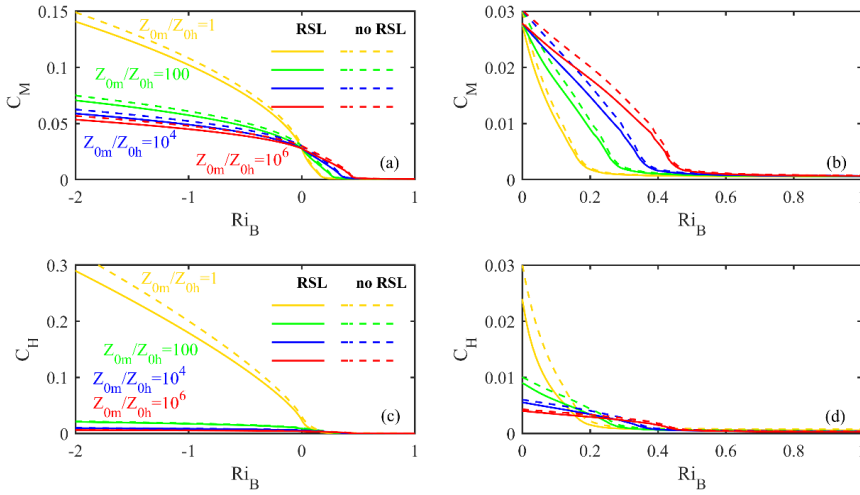


800  
801 **Figure 4.** The relationship between  $C_M(C_H)$  and  $Ri_B$  for different  $z_{0m}$  values and treatment of RSL. Solid lines:  
802 considering the RSL effect; dotted lines: without the RSL effect.  
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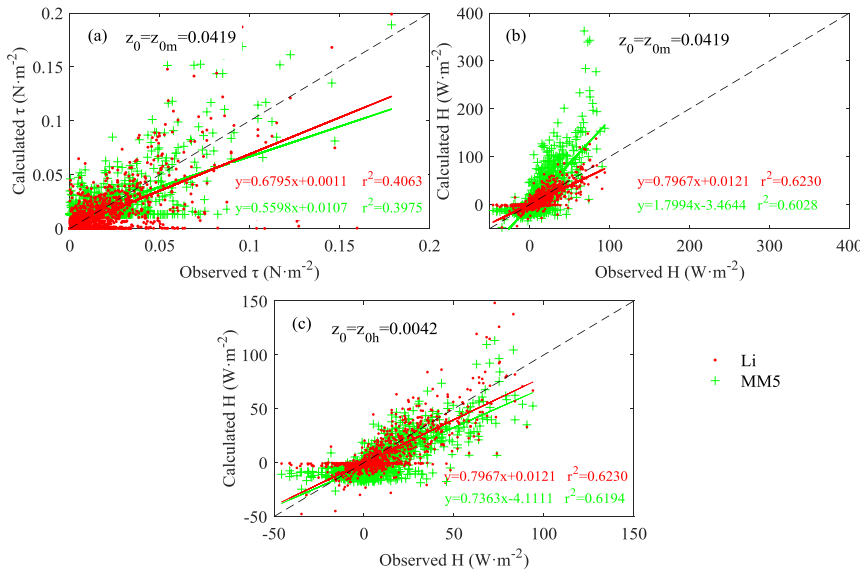
805

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

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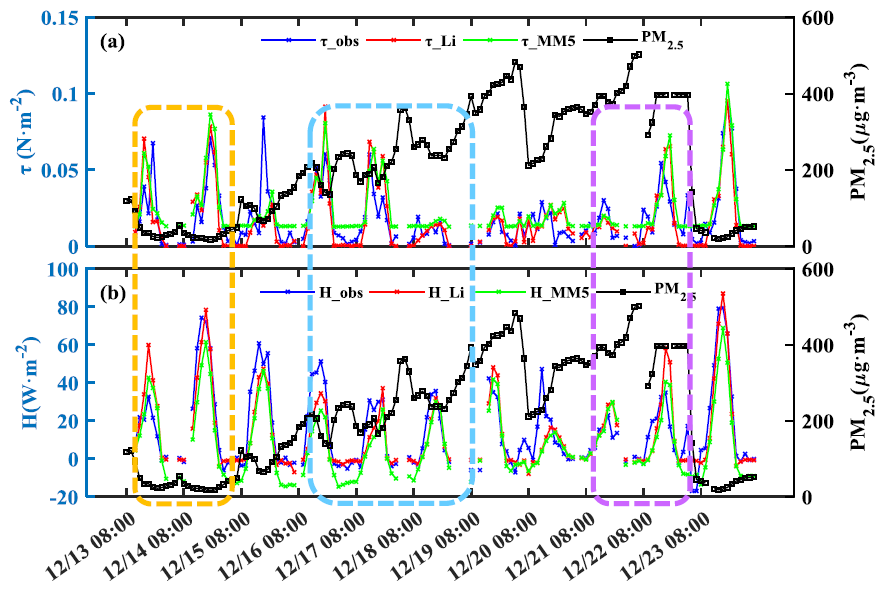
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811

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

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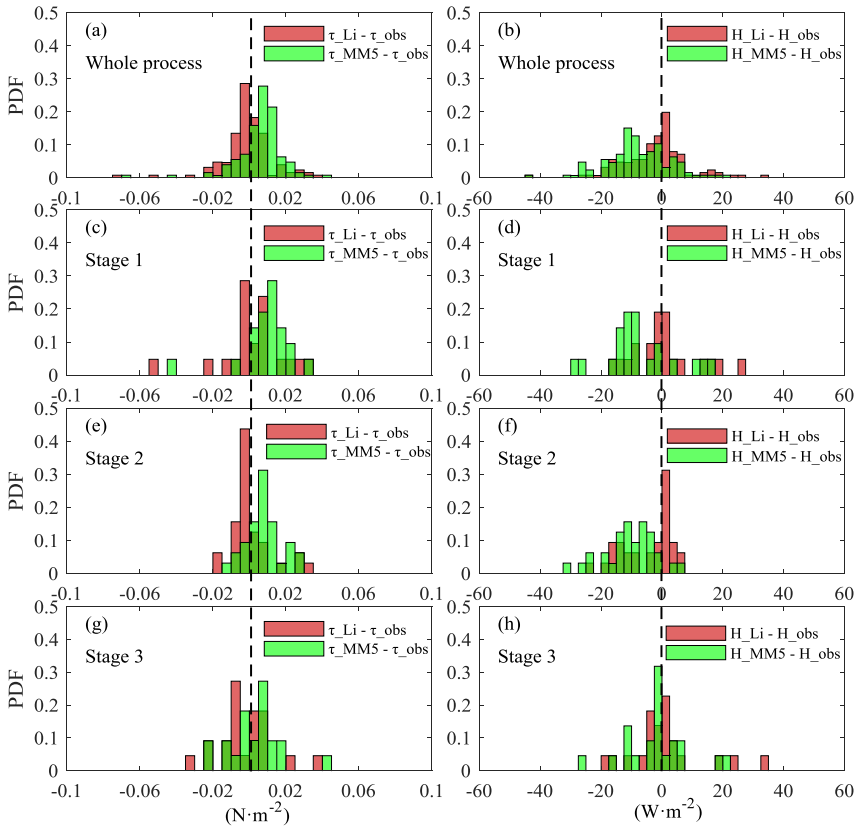
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817 **Figure 7.** Variations of hourly turbulent fluxes and **observed**  $PM_{2.5}$  at **GCGucheng** station in daytime. (a) Momentum fluxes  $\tau$   
 818 (blue line: observations; red line: the Li scheme; green line: the MM5 scheme) and  $PM_{2.5}$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

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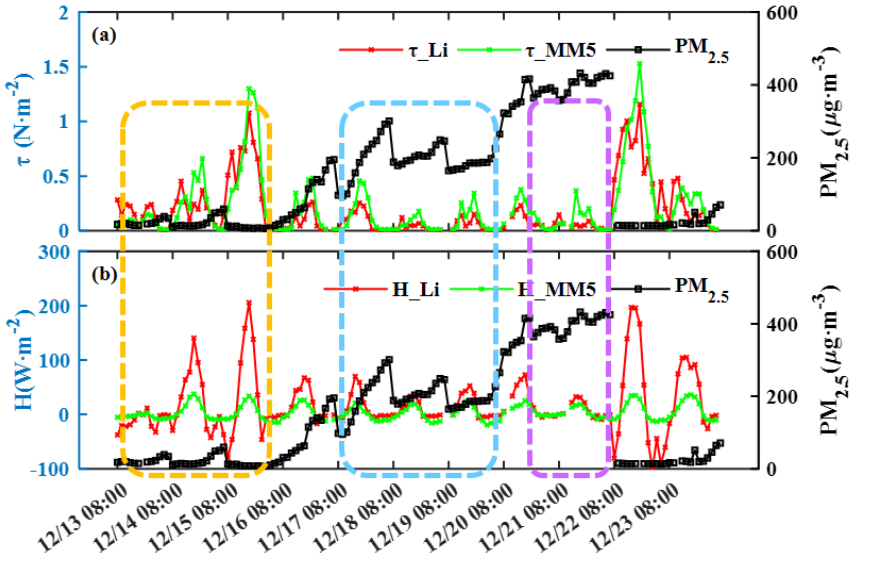
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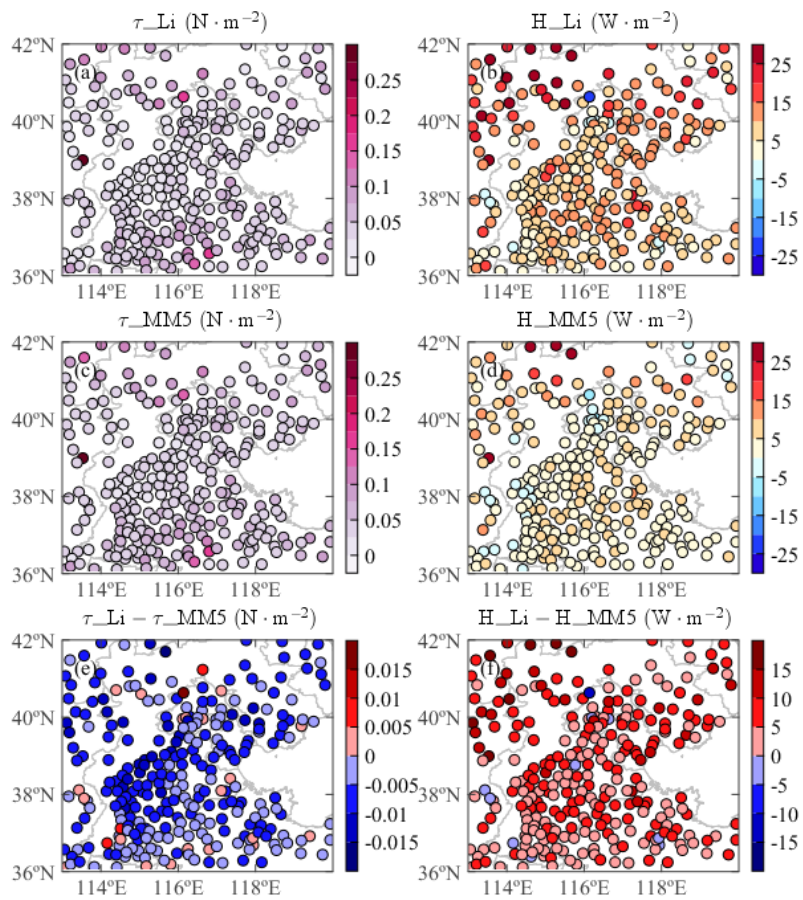
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825 **Figure 8.** Probability distribution functions (PDF) of the difference between calculated fluxes (momentum fluxes: left;  
 826 sensible heat fluxes: right) by using two schemes (the Li scheme: red bars; the MM5 scheme: green bars) and observations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



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



830

831 **Figure 10.** The mean momentum and sensible heat fluxes calculated by using two schemes (a-b: the Li scheme; c-d: the  
 832 MM5 scheme) and their difference (e: difference of the momentum fluxes; f: difference of the sensible heat fluxes) in  
 833 Jing-Jin-Ji region during the haze episode (December 13 to 23, 2016).

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