The Effects of Different Planetary Boundary Layer Schemes on the Meteorological and Environmental Elements in winter stable weather of Shenyang

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Abstract. Two planetary boundary layer schemes (YUS and MYJ) in the WRF-CMAQ model, are selected for sensitivity simulation, and the simulation capabilities of different planetary boundary layer schemes to meteorological elements and PM2.5 concentration distribution are analyzed from December 17th to December 20th in 2016. The results show that using the YSU and MYJ schemes can well simulate the spatial distribution and diurnal variation characteristics of temperature, wind speed and PM2.5 concentration on the ground under the background of stable weather in winter. It is sensitive to temperature, wind speed and PM2.5 concentration on the ground using different planetary boundary layer parameterization schemes. The simulated wind speed is relatively large, and the maximum deviation can reach about 2m/s. The deviation of wind speed using the MYJ scheme is relatively smaller than YSU, which is closer to the real value. There has a lower PM2.5 concentration value using YSU than MYJ at night, however the daytime (mainly from 11:00 to 18:00) YSU scheme is relatively higher than MYJ. The deviation of PM2.5 concentration on the ground using the MYJ scheme is relatively smaller than YSU, and the characteristics of daily variation is closer to the real situation. Overall, the MYJ scheme is better than YSU in air pollution simulation.

1. Introduction
Planetary boundary layer schemes is not only an important part of meteorological model, but also an important basis for air pollution model\cite{1-4}. The influence of atmospheric boundary layer on pollutant diffusion has been analyzed by using different planetary boundary layer schemes, which has attracted serious attention of researchers.

Extensive research has been carried out at home and abroad to study the effects of different boundary layer schemes on the simulation of wind, temperature field and pollutant diffusion in the boundary layer. For example, different boundary layer schemes have been used to simulate boundary layer structure in summer \cite{5}, surface wind speed and surface temperature \cite{6}. It is showed that the model does not fully consider the resistance effect of urban buildings, and the simulated deviation of surface wind speed is large, however it has good ability to simulate the daily variation characteristics
of surface temperature. Most foreign researchers believe that the simulated effect using the non-local closure scheme is superior to the local closure scheme in the unstable stratification. Pleim believes that the height of the atmospheric boundary layer can be well simulated in the afternoon using the ACM2 combination scheme\[7\]. Zhang et al. \[8\] found that the wind speed simulated by each scheme in the daytime is relatively high in Mexico City in March 2006, and the YSU scheme has a good effect on ground temperature in the daytime. Cheng et al. \[9\] analyze the results of air quality simulation in Taiwan of China, and believe that each boundary layer parameterization scheme has different effects on the distribution of O\(_3\) concentration under different weather systems. Ying Wang et al. \[10\] believe that the locally closed MYJ scheme can better simulate the daily variation characteristics of the bottom temperature in stable boundary layer in Lanzhou, while the temperature profile simulated by the ACM2 scheme in the daytime is better than the MYJ and YSU schemes. It is found that the results reveal that the differences between the simulations of temperature at 2 m level during the daytime using four PBL schemes is negligible by Wenxing Jia\[11\]. Wenxing Jia\[12\] et al found that the nonlocal closure schemes (MRF, YSU and SH schemes) are more suitable for unstable stratifications. Due to the nonlocal effects, these schemes will produce stronger turbulent mixing.

Although some consensus has been reached on the influence of the boundary layer process on the concentration distribution of pollutants, the research on the advantages and disadvantages of different schemes and their applicability is not enough, and there is not much research on the effect of concentration distribution. Meanwhile there are few researches on the effects of different planetary boundary layer schemes on the meteorological and environmental elements in Shenyang. In this paper, two planetary boundary layer schemes (YUS and MYJ) in the WRF-CMAQ model are selected for sensitivity simulation, and the simulation capabilities of different planetary boundary layer schemes to meteorological elements and PM2.5 concentration distribution is analyzed. Then we hope that it can provide a reference for the parameter selection in the prediction of air quality.

2. The data and the selection of weather case
A case of stable weather in winter is selected in Shenyang. During the period of from December 17th to 20th in 2016, there is a heavy pollution process with an air quality index of (AQI) more than 200 and fine particulate matter concentration (PM2.5) more than 200\(\mu\)g/m\(^3\). Because the weather situation is relatively stable (figure omitted), the wind speed is relatively small, and the pollutants are difficult to spread effectively, the air is always heavily polluted form the evening of 18th to the evening of 19th. The air pollutant concentration observation data comes from Liaoning Environmental Monitoring Center Station, and the meteorological data comes from Liaoning Meteorological Information Center.

3. The introduction of model and experimental scheme
3.1. WRF-CMAQ model settings
The mode system of WRF-CMAQ model is used in the study. WRF model used in the simulation test is the 3.4.1 version. The main part of CMAQ model is the CCTM module, which is the 4.7 version. The output result of the WRF model is input into MCIP (The Meteorology-Chemistry Interface Processor) and converted to the format file(NETCDF), which provide the meteorological background field for the CMAQ model.

The initial field and the boundary data of the WRF model provided by the US NCAR/NCEP in the study are the reanalyzed data with the resolution of 1°×1° center and the time interval of 6 hours. There is double nested, and the parent and child domains have the same center, which center coordinates are 41.73°N, 123.45°E in the simulation test. The grid spacing of coarse grid and fine grid are 3 km and 1 km, respectively, and the numbers of grid points are 92 × 80 and 82 × 73, respectively. The number of vertical layers is 23. The Noah land surface scheme is selected among the land surface processes. The WSM 6 classification harem scheme is selected among the microphysical parameterization processes. The cumulus convection parameterization scheme is selected among the Kain-Fritsch schemes. The RRTM long wave radiation scheme and the Dudhia short wave radiation
scheme are selected. The CMAQ model can simultaneously simulate the transport and conversion processes of multiple pollutants, and handle complex air pollution situations, such as ozone, particulate matter, poisons, acid deposition, and visibility. The CMAQ model includes many modules, the most important one among which is the chemical transport module (CCTM). There are two chemical conversion mechanisms in the CMAQ modes, which are CB4 and RADM2. You can also modify these mechanisms or use new chemical mechanisms in the CMAQ modes. In this study, the RADM2 chemical mechanism is used, and the grid setting in the horizontal direction is the same as the WRF setting. The model is divided into 12 layers in the vertical direction, and the σ values from the lower layer to the upper layer are 1, 0.99, 0.98, 0.97, 0.96, 0.8, 0.7, 0.6, 0.5, 0.3, 0.2, 0.1, and 0, respectively. In this study, the WRF-CMAQ model system is used to simulate. The simulation period is selected for 72 hours in total from 20:00 on December 17, 2016 to 20:00 on December 20, 2016 (Beijing time) and the simulation results are output once an hour.

3.2. The list of emission sources
The list of anthropogenic emission sources comes from MEIC (Multi-resolution Emission Inventory for China) in the CMAQ model, which space resolution is 0.25°. The list of emission sources covers 10 major atmospheric pollutants, greenhouse gases and more than 700 man-made emissions sources. The emissions data come from 5 sectors including power, industry, civil, transportation and agriculture, which can provide monthly gridded emission inventory. The study is based on MEIC V1.0, and selects the 2010 emission data and the appropriate chemical mechanism, and establishes the emission data required by the air quality model.

3.3. The parameterization scheme of planetary boundary layer
The parameterization of planetary boundary layer is aimed to describe the turbulent flux at the sub-grid scale. The expression method of turbulent flux in the numerical model is called the turbulent closure problem. The WRF-CMAQ provides three parameterization schemes of planetary boundary layer options, which are YSU, MYJ and ACM2 scheme (Table 1). Two parameterized schemes, YUS and MYJ, are selected for sensitivity simulation, and the simulation capabilities of different PBL schemes to meteorological elements and concentration distribution of PM2.5 is analyzed in the study.

| Scheme | The temperature at the bottom of the cloud | The treatment method about turbulent mixing in planetary boundary layer | The height at the top of the planetary boundary layer |
|--------|------------------------------------------|------------------------------------------------------------------------|---------------------------------------------------|
| YSU    | Non-local parameter of Tier 1             | K profile and reverse gradient term. Calculate the exchange coefficient using similarity theory TKE diagnosis. | Critical Richardson number |
| MYJ    | Local parameter of Tier 1.5              | Calculate exchange coefficient using Kolmogorov turbulence theory      | Critical turbulent energy |
| ACM2   | Non-local and local parameter            | Calculate the exchange coefficients using the turbulent exchange formulas of wind shear and local geographic Chason | Critical Richardson number |

4. Results and discussion
4.1. The analysis of simulation results of surface meteorological elements
It can be seen from Figure 1 that the two groups of experiments can simulate the characteristics of the diurnal variation of surface temperature. However, due to the different treatment of the physical
processes in the planetary boundary layer, the difference in surface turbulent transport will cause the significant difference in the simulated temperature in the two groups of experiments using the same land surface parameters. Therefore, it is sensitive to ground temperature using different planetary boundary layer parameterization schemes. The average temperature difference between the two groups of experiments on the ground temperature in the daytime is 1.3°C on average, which is generally higher at night with the average value 1.8°C, and could reach 2.2°C at most. Overall, the temperature deviation of the MYJ scheme is relatively small, which is closer to the real value.

![Figure 1](image1.png)  
**Figure 1.** The comparison of daily variation between simulated and observational ground temperature from 20:00 December 18th to 20:00 December 19th in Shenyang

Figure 2 shows that the variation of ground wind speed is more complicated about. During the period from 20:00 December 18th to 20:00 December 19th, the ground wind speed is weak, and its characteristics of daily variation about the ground wind speed are well simulated using the parameterization schemes YSU and MYJ respectively. The speed of wind starts to increase in the morning and reaches its maximum at noon. The simulation results of the two groups of tests are close to the real conditions. The simulation error mainly comes from the daytime. The simulated wind speed is relatively large, and the maximum deviation can reach about 2m/s. Overall, the deviation of wind speed using the MYJ scheme is relatively small, which is closer to the real value.

![Figure 2](image2.png)  
**Figure 2.** The comparison of daily variation between simulated and observational wind speed from 20:00 December 18th to 20:00 December 19th in Shenyang
4.2. The analysis of simulation results of ground level PM2.5 concentration

In order to test the simulation effect of different parameterization schemes for PM2.5 concentration on the ground, the data from air quality monitoring stations in Shenyang is used to compare with the simulated results obtained using YSU and MYJ experiments (figure 3). It can be seen that the two groups of experiments (YSU and MYJ) can well simulate the daily variation characteristics of the PM2.5 concentration on the ground. The PM2.5 concentration reaches the maximum at about 23:00 at night, and then decreases rapidly. It reaches the minimum at about 3:00 in the morning, and reaches the second peak after 11:00 during the day. Overall, the PM2.5 concentration on the ground is slightly higher at night than in the daytime. Due to the different descriptions of the turbulent mixing in the planetary boundary layer, the difference in the planetary boundary layer process will lead to significant differences in the simulation results of two groups of experiments about PM2.5 concentrations under the same conditions of emission intensity and surface parameters. The simulation of PM2.5 concentration is sensitive to the parameterization schemes of planetary boundary layer.

The simulated results of PM2.5 concentration at night in the two groups of experiments are better than in the evening, which are higher at about 5:00 and basically lower in other periods. This may be related to the simulated wind speed which is higher than the real value. Through the comparison of the two groups of experiments, there has a lower PM2.5 concentration value using YSU than MYJ at night, however the daytime (mainly from 11:00 to 18:00) YSU scheme is relatively higher than MYJ. The simulated relative deviation of the two groups of experiments is smaller when the pollution level is higher. It is larger when the pollution level is lower. This may be related to the uncertainty of the spatial distribution about the emission source and the emission time, etc(table 2).

Figure 3. The comparison of daily variation between simulated and observational PM2.5 concentration from 20:00 December 18th to 20:00 December 19th in Shenyang

Table 2. The errors statistics of ground PM2.5 concentration using two groups of experiments (unit: mg / m$^3$)

| Parameter                | YSU  | MYJ  |
|--------------------------|------|------|
| Mean absolute deviation  | 0.042| 0.037|
| Standard deviation       | 0.053| 0.048|
5. Conclusions and discussions.

(1) The two planetary boundary layer schemes (YSU and MYJ) in the WRF-CMAQ model can well simulate the spatial distribution and diurnal variation characteristics of temperature, wind speed and PM2.5 concentration on the ground under the background of stable weather in winter.

(2) It is sensitive to ground temperature and wind speed using different planetary boundary layer parameterization schemes. The average temperature difference between the two groups of experiments on the ground temperature in the daytime is 1.3°C on average, which is generally higher at night with the average value 1.8°C, and could reach 2.2°C at most. The simulation error mainly comes from the daytime. The simulated wind speed is relatively large, and the maximum deviation can reach about 2m/s. Overall, the deviation of wind speed using the MYJ scheme is relatively small, which is closer to the real value.

(3) Due to the different descriptions of the turbulent mixing in the planetary boundary layer, the difference in the planetary boundary layer process will lead to significant differences in the simulation results of the two groups of experiments about PM2.5 concentrations under the same conditions of emission intensity and surface parameters. Overall, the deviation of PM2.5 concentration on the ground using the MYJ scheme is relatively smaller than YSU, and the characteristics of daily variation is closer to the real situation.

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