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Study on the applicability of key parameters from dust emission scheme in WRF/Chem over northwestern China

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Abstract. In order to more accurate quantitative simulation and forecast of sandstorm in northwest China, in this paper, the dust process occurred in northwest China was simulated by using the WRF/Chem model coupling of Shao2004 dust emission parameterization scheme. The influence of key parameter C in Shao2004 scheme is analyzed set at different values on simulated spatial and temporal dust concentration, estimated vertical dust flux and estimated PM_{10} and $PM_{2.5}$ concentration of six stations in northwest China. And by comparing the concentration of PM concentration observed at the sites, the results were listed as: Parameter C has an significant influence on the simulation dust scope and maximum center value of dust concentration and vertical dust flux; Different C values can well simulate the variation trend of PM_{10} and $PM_{2.5}$ concentration in dust weather, but only when the C value set as 1, this model can more accurately simulate the change of PM_{10} and $PM_{2.5}$ concentration in the dust process in northwest China.

1. Introduction

Dust storm is a very complicated and important weather process, often occurring in northwest China, and it can greatly increase the concentration of ambient particulate matter resulting in worse atmospheric visibility, serious atmospheric pollution and human health risks[1-3]. In addition, dust aerosols also have important impacts on global and regional climate system[4-6]. To understand the emission, transmission, range of dust-related processes and dust effects on atmospheric environment and climate, a series of sandstorm monitoring and prediction systems have been developed and applied to simulation and forecast it[7-11]. Those models, such as the Nested grid air quality prediction model system (NAQPMS)[12]and the sandstorm model GRAPES_SDM coupling the Global/Regional Assimilation and Prediction Enhanced System (GRAPES)[13,14], simulate and forecast sandstorm weather in northwest China with an accuracy of quantitative simulation needed to be improved[14]. Beyond that, most dust forecast models based on parameterization schemes simulate the dust weather in some degree accompanied by high uncertainties like GOCART, DEAD, MASINGAR, COAMPS, CEMSYS5, CFORS, DREAM[15-20].

The dust emission parameterization scheme is the key to accurately simulating and forecasting sandstorm to which the key lies in the calculation of vertical dust flux on the surface. Numerous studies for describing dust emission parameterization scheme were proposed at home and abroad[21-23]. According to physical significance of the surface dust flux model, the dust emission parameterization scheme was classified into three types, namely, α scheme, β scheme and γ scheme. Among them, γ scheme in view of three dust emission mechanisms (entrainment of air drag force、 saltation bombardment and aggregate disintegration) is a spectral scheme based on the physical process of wind erosion[24-26]. Further, a size-resolved dust emission equation was proposed by supposing that particles are divided into I particle-size intervals which was further simplified in Shao et al. (2004) . Thus, the dust emission parameterization scheme proposed by Shao 2004 (hereinafter S04) was proposed based on the three kinds of dust emission mechanisms mentioned above and particle size spectrum distribution, which in a sense is more practical on account of considering as many factors as possible so far. However, for reaching a comparable higher accuracy, key parameters in the vertical sand flux equation, including soil plasticity pressure p and dimensionless coefficient c_y, weight factor γ related to the viscosity of sand with different particle sizes, and parameter C related to horizontal sand flux studied in this paper, have high localization applicability research value[27]. Through many simulation experiments and comparisons with the observed data in northwest China, the influence of key parameters on the dust emission parameterization scheme can be found, and the most appropriate values in northwest China can be obtained, which is of great value for improving the service capacity of sandstorm monitoring and prediction in northwest China. The constant C is the parameter related to horizontal sand flux which reflects the degree of saltation and creep and makes great contribution to vertical dust flux, and the value of horizontal sand flux is linearly proportional to the variable parameter C[19,28]. Therefore, finding the value of parameter C suitable for northwest China will greatly improve the accuracy of this model in simulating dust weather in northwest China.

In this paper, through the WRF/Chem model coupling S04 scheme, the estimated dust mass concentration and vertical dust flux in a typical case of sand-dust weather were analyzed when the parameter C related to the horizontal sand flux were taken as 1, 2 and 2.6, respectively. Meanwhile, compare simulated results with the measured particulate matter mass concentration to find the impacts of parameter C on dust simulation and the more suitable value of parameter C in S04 scheme for northwest China.

2. Data, model and experiment design

2.1 Observation data
A model simulation was conducted for two severe Asian dust events. To study the first one, hourly monitoring data of $PM_{2.5}$ and PM_{10} at six cities in northwest China (Karamay, Jiayuguan, Jinchang, Baotou, Lanzhou and Yinchuan) in 23-25 April 2014 were needed.

2.2 Dust model
The improved WRF/Chem model, coupling the Weather Research Forecast model (WRF) with the chemical module about atmospheric chemical processes (Chem), makes an online coupling of the atmospheric model and chemical module in temporal and spatial. The processes of dust emission, transmission and deposition are considered in WRF/Chem V3.0 and WRF/Chem above V3.0, which can be used to simulate dust events. Kang et al. (2011) coupled the S04 scheme to the WRF/Chem V3.2. The WRF/Chem model based on the S04 scheme has been widely applied to the simulation of dust weather in northwest China[29,30]. In this paper, we use the WRF/Chem V3.6.1 coupling the S04 scheme to estimated dust emission in northwest China. The dust emission parameterization (S04 scheme) was described as follow:

For a particle with a size di, the vertical sand flux by saltation can be estimated using the equation (1) as following:

$$F(i,j) = c_y \eta_{fj} \left[(1-\gamma) + \gamma \frac{p_m(d_j)}{p_f(d_j)} \right] \frac{Q(i)g}{u_*^2} (1 + \sigma_m) \qquad (1)$$

where c_y is a dimensionless coefficient; η_{fj} is the mass fraction of dust particles; γ is a weight factor related to the viscosity of sand particles of different sizes; g is the acceleration of gravity; u_* is the friction velocity; $pm(d_j)$ and $pf(d_j)$ are known as minimally disturbed particle size distribution and fully disturbed particle size distribution, respectively; p(d) is represented by

$$p(di) = \gamma p_m(di) + (1-\gamma)p_f(di) \qquad (2)$$

$$\gamma = \exp[-(u_* - u_*)3] \qquad (3)$$

σ_m is the effective bombardment rate of sand particles, and its expression is

$$\sigma_m = 12u_*^2 \frac{\rho_b}{p} \left(1 + 14u_* \sqrt{\frac{\rho_b}{p}} \right) \qquad (4)$$

Where ρ_b is the soil bulk density，p is the soil plastic pressure. Q(i) is the flux of bombarding sand with particle size (horizontal flux of sand grain) which is expressed as

$$Q(i) = c\frac{\rho_a}{g} u_*^3 \left[1 - \frac{u_{*t}^2(d_j)}{u_*^2} \right] \qquad (5)$$

where C is the parameter related to horizontal sand flux and also the key parameter to be discussed in this paper. The vertical saltation flux for all particle sizes can be estimated by

$$F = \int_{d_1}^{d_2} F(d_i) \, p(di)\delta di \qquad (6)$$

where d_1 and d_2 are the lower and upper size limits, respectively, of the saltating particles.

2.3 Experiment design
The first step is to reset the key parameter C (related to the horizontal sand flux) of vertical sand flux equation in S04 scheme at 1, 2 and 2.6, respectively. Then, the dust event was simulated by WRF/Chem which happened from 20:00 (BJS) on 23 April to 20:00 (BJS) on 25 April, 2014. The area to be simulated mainly contains northwest, north and central China of which the map has 140 grid points in the zonal direction and 80 grid points in the meridional direction along with a horizontal resolution of 27km and 48-layers vertical atmosphere, with central point of the simulated area set at (96 °E, 40 °N) (Figure 1). The initial and boundary conditions of the meteorological driven field were derived from the global reanalysis data with the resolution of 1°×1° updated every 6 hours by NCEP. The initial and boundary conditions for the chemicals were the simulation output results every 6 hours from the MOZART-4 model. Twelve cases in each dust event were simulated but only the simulation results at 13:00 (BJS) per day were chose to analyze.
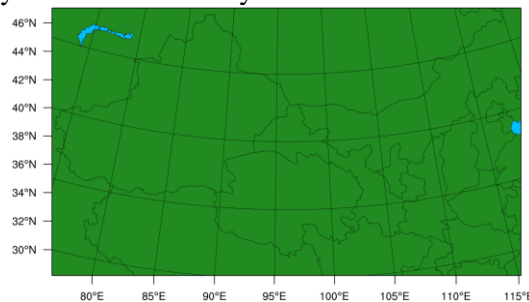

Figure 1 Simulation area diagram (mainly in northwest China)

3. Results and analysis

3.1 The synoptic circulation situation for dust events
Based on the global reanalysis data of NCEP, the evolution process of the circulation situation for dust event in 23-25, April 2014 was shown in Figure 2. As seen from the geopotential altitude field on the

23rd, a large trough was situated in the northeast of Xinjiang province. Due to the large trough, there was windy weather in the middle and eastern Xinjiang, resulting in a beginning of dust emissions which would affect most of Xinjiang. Constantly, the trough moved eastward to the southern Mongolia on the 24th and a low-vortex appeared at this time with a low-pressure center (53°N, 105°E), while the sandstorm region has shifted from Xinjiang to the southern Mongolia and northern Inner Mongolia on account of a frontal zone located in south of Lake Baikal, between south-central Mongolia and northern Inner Mongolia. The low-vortex developed rapidly eastward on the 25th with the low-vortex center located at (55°N, 115°E), and the frontal area has been reduced, mainly affecting the southeastern Mongolia and north-central Inner Mongolia which were mainly dust emission areas.
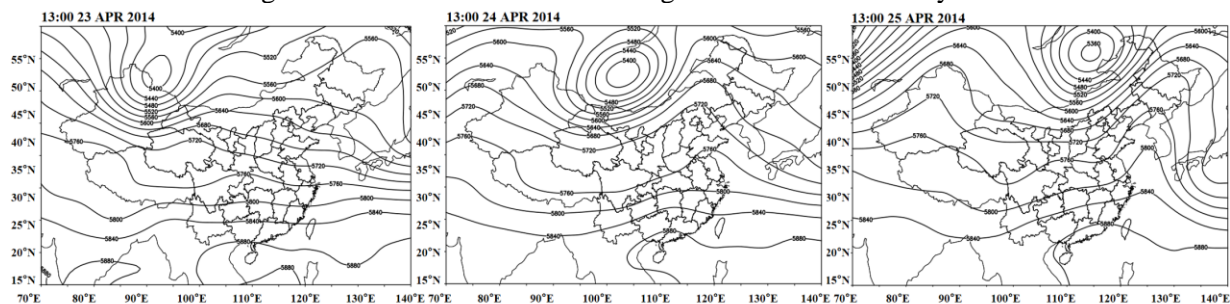

Figure 2   500 hPa geopotential altitude filed at daily 12:00 (BJS)
in 23-25, April 2014 from NCEP reanalysis data (units:gpm).

3.2 Effect of key parameter C on dust emission simulation

3.2.1 Effect on estimated dust concentration
Figure 3 shows the regional simulation results of dust concentration at 13:00 (BJS) from 23 to 25 April 2014, corresponding to different C values. Under the same constant C (seeing horizontally), dust concentration range gradually expanded with time. It was mainly in the whole Xinjiang province on 23rd when the dust concentration maximum reached the highest. On April 24, dust event happened in the whole northwest China and constantly spread to the northern Tibet and the Sichuan basin on 25th. According to the numerical simulation results from WRF/Chem, the dust concentration maximum sharply decreased from 151655 $\mu g \cdot m^{-3}$ on 23rd to 20664.74 $\mu g \cdot m^{-3}$ on 24th and increased slowly to 38949.59 $\mu g \cdot m^{-3}$ on 25th , which was the simulation results corresponding to the parameter C of 2.6 shown in Figure 3a-c. From the vertical perspective, with the decrease of C value, the simulation range of dust concentration slightly shrunk accompanied by a decline of dust concentration maximum whose overall position did not change. Taking the numerical simulation results on 23rd as an example (Figure 3a, d and g), the dust concentration maximum decreased significantly from 151655 $\mu g \cdot m^{-3}$ (a) to 116657.7 $\mu g \cdot m^{-3}$ (d) and finally to 58328.86 $\mu g \cdot m^{-3}$ (g) along with a decline of C value. The temporal and spatial variation trends of estimated dust concentration for different constant C was consistent. Thus, the change of C value did have a great impact on simulated dust concentration, that is, the larger the constant C was, the stronger the simulated dust weather phenomenon would be.
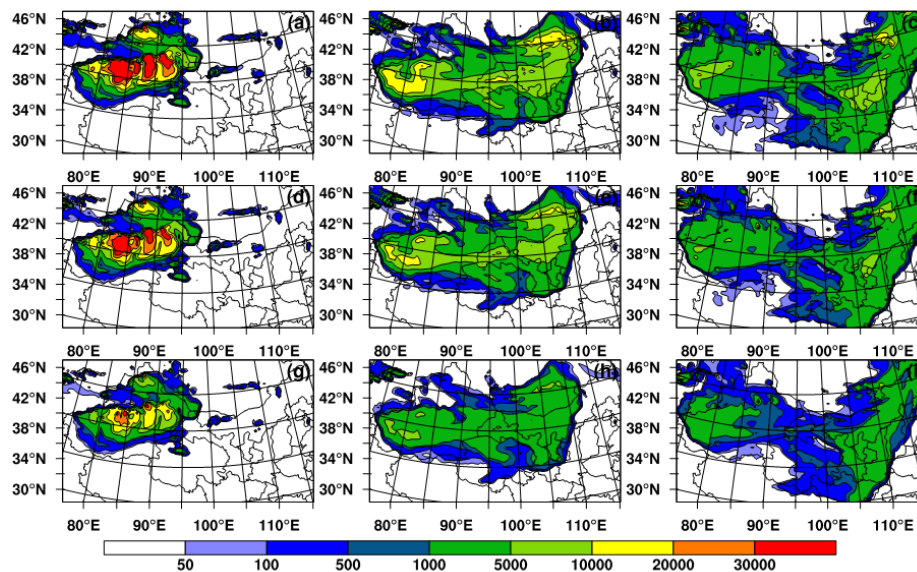
Figure 3 Simulation diagram of dust concentration with different C values at 13:00 in April 23-25, 2014 (units: ug·m-3, time: BJS). The dust concentration range at 13:00 from 23 to 25, April 2014 with the constant C of 2.6 was shown in (a)-(c); The dust concentration range at 13:00 from 23 to 25, April 2014 with the constant C of 2 was shown in (d)-(f); The dust concentration range at 13:00 from 23 to 25, April 2014 with the constant C of 1 was shown in (g)-(i).

3.2.2 Effect on estimated vertical dust flux

Figure 4 showed the regional simulation results of vertical dust flux at 13:00 (BJS) from 23 to 25 April 2014, corresponding to different C value. Under the same constant C (seeing horizontally), the simulation range of the vertical dust flux changed similarly comparing with dust emission analyzed above. It mainly distributed in the eastern Xinjiang on 23rd when the vertical flux maximum reached the highest and located in central Xinjiang, followed by a constant eastward movement. The vertical flux simulation range reach maximum on 24th, mainly distributed in northwestern Gansu province, south Mongolia, and north of Inner Mongolia. While the simulation range significantly decreased on 25th, and its overall position moved eastward, mainly distributed in southeast Mongolia. The simulation maximum center of vertical dust flux has been transferred from mid-east Xinjiang to southwestern Mongolia and to the border of the middle of Inner Mongolia and Mongolia, of which the value decreased from 33438.7 $\mu g \cdot m^{-2} \cdot s^{-1}$ on 23rd to 2449.164 $\mu g \cdot m^{-2} \cdot s^{-1}$ on 24th to 8185.144 $\mu g \cdot m^{-2} \cdot s^{-1}$ on 25th (taking results in Figure 4 a-c as an example). Seeing vertically, the simulation range of vertical dust flux had no obvious change consistent with the overall position of the flux maximum center. Whereas the vertical dust flux maximum decreased significantly from 33438.7 $\mu g \cdot m^{-2} \cdot s^{-1}$ (a) to 25722.07 $\mu g \cdot m^{-2} \cdot s^{-1}$ (d) and finally to 12861.04 ug·m-3 (g) with a decline of C value. The temporal and spatial variation trends of estimated vertical dust flux for different constant C was consistent. It's noted that the uncertainty of parameter C have a great impact on the vertical dust flux with a direct effect on the horizontal sand flux which was as same as the dust emission condition discussed above.
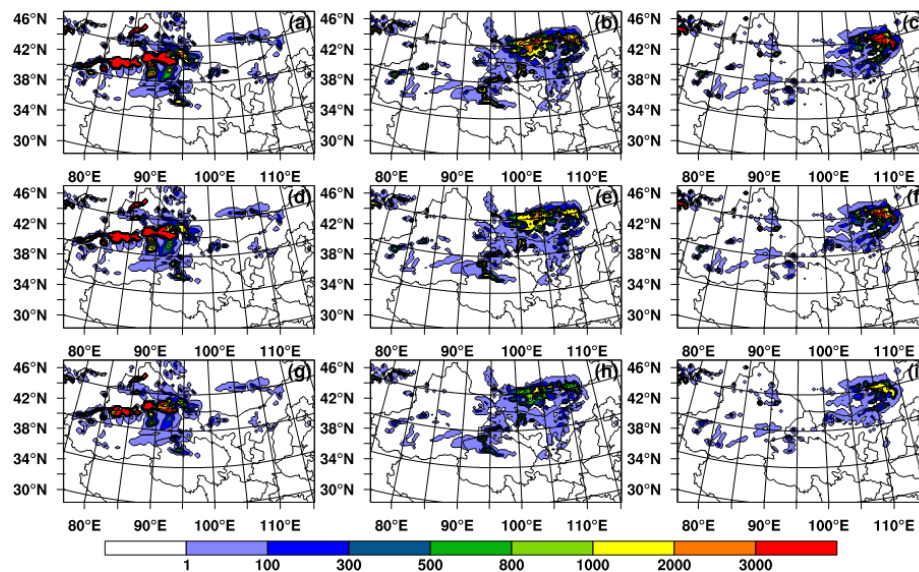
Figure 4 Simulation diagram of vertical dust flux with different C value at 13:00 in April 23-25, 2014 (units: μg·m-2·s-1, BJS). The vertical dust flux at 13:00 from 23 to 25, April 2014 with the constant C of 2.6 was shown in (a)-(c); The dust concentration range at 13:00 from 23 to 25, April 2014 with the constant C of 2 was shown in (d)-(f); The dust concentration range at 13:00 from 23 to 25, April 2014 with the constant C of 1 was shown in (g)-(i).

3.3 Comparison of estimated PM$_{2.5}$ and PM$_{10}$ concentration with those observed

The comparison of PM$_{2.5}$ and PM$_{10}$ concentration observed in six cities of northwestern China (Karamay, Jiayuguan, Jinchang, Baotou, Lanzhou and Yinchuan) during the dust weather process (in 23-25, April 2014) with the simulated results of PM at parameter C values of 1, 2 and 2.6 in S04 scheme were shown in Figure 5 and Figure 6, from which we can see the variation trend of PM$_{2.5}$ and PM$_{10}$ in dust weather can be simulated in consistent with those of observation. However, only parameter C was set at 1 can make both the simulated PM$_{2.5}$ and PM$_{10}$ concentration closest to those observed in six cities. The simulation results were most unreliable under parameter C of 2.6 that the estimated PM$_{2.5}$ and PM$_{10}$ concentration were generally 6 and 4 times higher than the observed values, respectively. When the value of parameter C was 2, the simulation result was approximately 3 or 4 times larger than the observed one. The conclusion obtained above was reliable in some degree since it concluded from comparison results of six cities in northwest China.
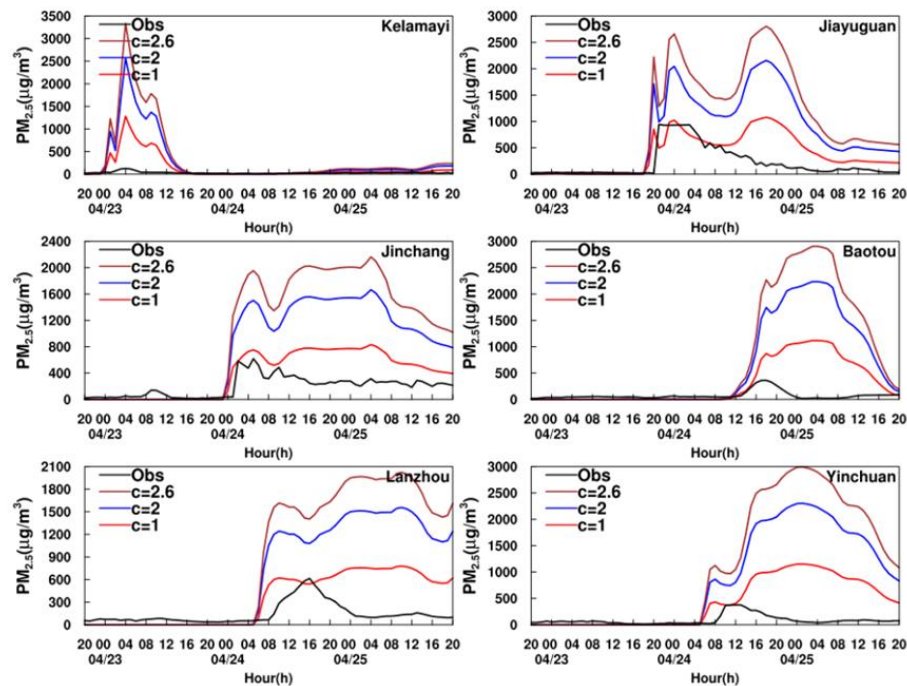
Figure 5 Comparison of the simulated results with observation data of $PM_{2.5}$ in northwest China (6 cities) under different C value
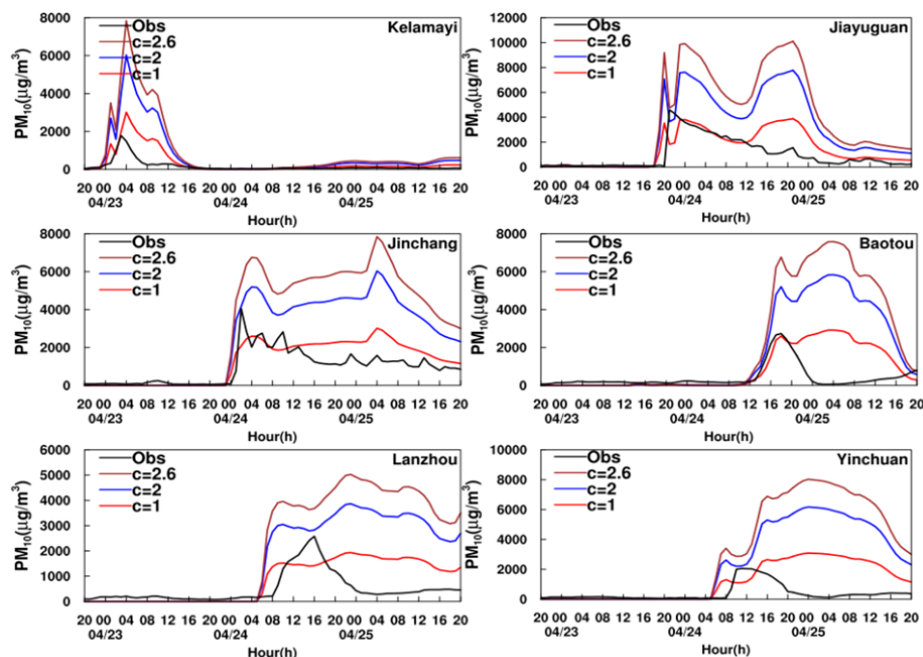

Figure 6 Comparison of the simulated results with observation data of PM_{10} in northwest China (6 cities) under different C value

4. Conclusion

By means of the WRF/Chem model coupled with S04 scheme, the sandstorm weather event in northwest China occurred in April 23-25, 2014 was simulated. The simulated results based on different parameter C (1, 2, and 2.6) and the comparison with the observed results were analyzed. In the comprehensive research and analysis from the surface (dust concentration range) to the lines

(vertical dust flux) to the point (station observation), we found the key parameter C related to the horizontal dust flux distinctly influenced the estimated dust not only in spatial distribution but also in dust concentration (vertical dust flux), really of great uncertainty. Compare the estimated particulate matter concentration with the measured ones to find the most suitable constant C for northwest China with some conclusions listed as follow：

(1) The simulated range of dust concentration decreased slightly with the decrease of C value while the maximum of dust concentration decreased significantly.

(2) There is no significant change in the simulation range and maximum center position of sand vertical flux, but the lower value of parameter C is, the maximum value of vertical dust flux was significantly lower.

(3) When the C value is set at 1, the model can more accurately simulate the variation of PM_{10} and $PM_{2.5}$ concentration during the dust process.

In conclusion, the key parameter C in the vertical sand flux equation can have a great influence on the simulated dust weather. The larger the C is, the easier it is to make a dust emission, and the larger the area affected by the dust will be. The accuracy and applicability of the simulation process of dust weather in northwest China is most applicable with parameter C of 1. The S04 scheme still has some important variable parameters needed to further study the uncertainty as well as their influence on each other, and find out the value of these parameters most suitable for northwest China, which can greatly increase the forecast accuracy and simulation.

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