Research on numerical simulation technology about regional important pollutant diffusion of haze

To cite this article: Boying Du et al 2018 IOP Conf. Ser.: Earth Environ. Sci. 121 032049

View the article online for updates and enhancements.
Research on numerical simulation technology about regional important pollutant diffusion of haze

Boying Du, Yunfeng Ma, Qiangqiang Li and Qi Wang, Qiongqiong Hu and Yushan Bian

Shenyang Aerospace University-College of Energy and Environment, Shenyang 110136, China

1 741033734@qq.com

Abstract. In order to analyze the formation of haze in Shenyang and the factors that affect the diffusion of pollutants, the simulation experiment adopted in this paper is based on the numerical model of WRF/CALPUFF coupling. Simulation experiment was conducted to select PM$_{10}$ of Shenyang City in the period from March 1 to 8, and the PM$_{10}$ in the regional important haze was simulated. The survey was conducted with more than 120 enterprises section the point of the emission source of this experiment. The contrastive data were analyzed with 11 air quality monitoring points, and the simulation results were compared. Analyze the contribution rate of each typical enterprise to the air quality, verify the correctness of the simulation results, and then use the model to establish the prediction model.

1. Introduction

According to the aerodynamic diameter, atmospheric particles can be divided into total suspended particulate matter, PM$_{10}$, fine particulate matter and so on. Compared with other larger diameter particles, the coarse particles in PM$_{10}$ are mainly human-derived particles and natural dust particles that easy to settle, and are easily blocked in the nasal and oral cavity. In addition, PM$_{10}$ accumulates more easily than large diameter particles such as PAN, PAH, and nitrates, sulfates and the like. Fine particles are mainly converted from polluting gases by complex heterogeneous chemical reactions or made from high temperature exhaust of supersaturated gaseous materials and then collide, aggregate, adsorb. The particles in the atmosphere can adsorb a large number of pollutants, bring out some sulfate, nitrate and so on, even breed more microorganisms. The problem of atmospheric environmental pollution is complicated and will be affected by many factors, such as the geographical terrain of the research area, the stability of the meteorological structure, the type of pollutants, the reaction between pollutants and the chemistry with each other. Zhong Sheng do air pollution treatment research that the main reason for air pollution is industrial waste gases, motor vehicle emissions in environmental engineering[1]. The calculation principle of three-dimensional Lagrange puff model based on unsteady state, then according to some local unique topography and climate conditions in real time localization to study, use of simulation technology has been simulated regional atmospheric pollution[2].

In the northeast region of China, where the coal is the main source of energy, the pollutants generated are mainly soot, NOx, SO$_2$. Shenyang as one of the three northeastern provinces in China of the city center, the main type of pollution is the coal smoke pollution, the use of CALPUFF model abased on the region's dust analysis must have a certain practical significance. In the terms of the use of the model, David M. Broday used the CALPUFF model to study the diffusion of point source
emission contaminants in the imaginary area of flat terrain[3] Elbir T established the Istanbul urban air quality management decision support system based on geographic information system (GIS), and mentioned the optimal use of the model[4].

2. Data and methods

2.1. Study area
Shenyang city is the northeast city of China, in the central of Liaoning Province, and Liaodong Peninsula is in the south of city, Changbai Mountain is in the north, located at latitude 41 degrees 48 minutes 11.75 seconds, longitude 123 degrees 25 minutes 25.18 seconds. The landform is dominated by plains, mountains and hills, while the hilly areas are concentrated in the southeast of the Shenyang area, which flows through the liaohe river, the hunhe river, the xiushui river and others.

In the simulation experiment of this paper, the mesh coordinates range of the study area (UTM): A (855km, 4459km), B (855km, 4859km), C (1250km, 4859km), and D (1250km, 4459km). The simulation number in the X Y direction are 200, the distance between the two grids is 2km, and the grid distribution is 400km*400km (As shown in Figure 1.); the vertical layer is set to 8 layers: 20m, 50m, 100m, 200m, 500m, 1000m, 2000m, 3000m.

![Figure 1. The 400×400 km range of simulated study grids chart.](image1)

![Figure 2. Distribution of the source of pollution.](image2)

2.2. Materials and methods
In this case, the PM$_{10}$ of the particulate pollutants in Shenyang area in 2016 was taken as the object of study. The data of particulate matter emission sources were collected, including the latitude and longitude, the size of emissions, the time of emissions, the way of emissions and so on. The paper collects detailed emissions data from 120 typical emission units that include the boiler heating industry, electroplating factories, engine manufacturing and the pollution units that have a large impact on the study area. The spatial distribution of pollution sources was created using the software Google Earth. The distribution location of the pollutant emission source is shown in figure 2.

The detailed parameters such as source, emission rate, and speed of pollution sources are shown in table 1. In order to simplify the experimental plan, refer to "Emission Standard of Boiler Air Pollutants" (GB13271-2014) to set the chimney height to 15 meters. accord to "Thermal Power Plant
FGD Engineering Specification Limestone/Lime-Gypsum Method" the chimney outlet temperature is set to 80°C[5, 6].

Table 1. Part of the pollution source detailed data.

| Pollution point | X(km)     | Y(km)     | Altitude (km) | Chimney height (m) | Temperature (K) | Emission rate (mg/s) |
|-----------------|-----------|-----------|---------------|-------------------|-----------------|----------------------|
| Point 1         | 527.472   | 4624.66   | 26            | 150               | 353             | 200.34               |
| Point 2         | 558.503   | 4618.83   | 100           | 150               | 353             | 340.56               |

Meteorological Element Field Data Selection, WRF modeling is often used in the use of mesoscale meteorological data, however, the feature resolution of WRF is large, which can’t be generated for high-resolution terrain surface features, so that leads to the roughness of WRF meteorological simulation results. Therefore, the CALMET weather diagnostic module can be used to further refine the initial generation of weather. Figure 3 is the simulated initial field of WRF.

Figure 3. WRF meteorological field nested map.

Figure 4. Monitor site space location distribution.

Terrain surface information is based on data from the US Geological Survey (USGS). Terrain data is 900 meters accuracy, land use type data is 1000m accuracy. Table 2 is the WRF weather simulation area design details.

Table 2. WRF weather simulation area design.

| Nested area | Grid points X×Y | Lattice distance Δ X, Δ Y | Integral step Δ t |
|-------------|-----------------|---------------------------|-------------------|
| Domain1     | 65×49           | 36km.36km                 | 3600s             |
| Domain2     | 91×61           | 12km.12km                 | 3600s             |
| Domain3     | 106×97          | 4km.4km                   | 3600s             |

Table 3. Simulation of experimental time in the study area.

| Time        | Year | Month | Day | Hour | Minute | Second |
|-------------|------|-------|-----|------|--------|--------|
| Start time  | 2016 | 3     | 1   | 00   | 00     | 00     |
| End time    | 2016 | 3     | 8   | 00   | 00     | 00     |

The data of the March event with early spring particle activity were selected as the experimental data and the simulation time listed in Table 3, because the value of PM$_{10}$ particles in March was relatively large compared with other months and the simulation results were more accurate. The selection of the contaminant diffusion step in the experiment can be customized according to the requirements. In this study, the step size is 3600s, that is, the length of one hour.
In the model of CALPUFF puff diffusion, the fundamental concentration equation of a single puff (puff) at a receiving point is\[7\]:

\[
C = \frac{Q}{2\pi \sigma_x \sigma_y} \exp\left[-d_u^2/(2\sigma_x^2)\right] \exp\left[-dc^2/(2\sigma_y^2)\right]
\]

\[1\]

\[
g = \frac{2}{(2\pi)^{3/2} \sigma_z} \sum_{n=0}^{\infty} \exp\left[-(H + 2nh)^2/(2\sigma_z^2)\right]
\]

\[2\]

Where, \(C\) is the ground-level concentration (g/m\(^3\)), \(Q\) is the pollutant mass (g) in the puff, \(\sigma_x\) is the standard deviation (m) of the Gaussian distribution in the along-wind direction, \(\sigma_y\) is the standard deviation (m) of the Gaussian distribution in the cross-wind direction, \(\sigma_z\) is the standard deviation (m) of the Gaussian distribution in the vertical direction, \(d_a\) is the distance (m) from the puff center to the receptor in the along-wind direction, \(d_c\) is the distance (m) from the puff center to the receptor in the cross-wind direction, \(g\) is the vertical term (m) of the Gaussian equation, \(H\) is the effective height (m) above the ground of the puff center, and \(h\) is the mixed-layer height (m).

In the course of the movement of the meteorological module, in addition to the calculation method of selecting the puff, the calculation model of the slug can be used, and the puff is slightly different in the small-scale integration step[8].

\[
C(t) = \frac{Fq}{(2\pi)^{3/2} \sigma_x \sigma_y} g \exp\left[-d_u^2 u^2/(2\sigma_x^2 u^2)\right]
\]

\[3\]

\[
F = \frac{1}{2} \left\{ \text{erf}\left[\frac{d_{a2}}{\sqrt{2} \sigma_y}\right] - \text{erf}\left[-\frac{d_{a1}}{\sqrt{2} \sigma_y}\right] \right\}
\]

\[4\]

Where, \(U\) is the average wind vector (m/s) in the study area; \(U'\) is wind speed (defined as: \(u = (u^2 + \sigma_v^2)^{1/2}\) = variance) (m/s); \(Q\) is for source strength (g/s); \(F\) is the "causality" function; \(G\) is vertical coupling factor.

**Figure 5.** Concentration contrast diagram.  **Figure 6.** Wind rose diagram.
3. Result and discussion

3.1. Numerical simulation and comparative analysis

Numerical simulation is mainly used to compare the variation of the concentration of $\text{PM}_{10}$ with the actual 11 monitoring points (The specific location shown in Figure 4) corresponding to the change of $\text{PM}_{10}$.

The result data of the model was output once per hour, and the data of 8 days was divided into four periods to analyze. The data of comparative analysis of Shenyang city from March 1 to March 8th of 2016 are drawn into a chart of lines. (To take Artillery Academy as an example and the simulation results shown in Figure 5.)

It can be seen from the above: four comparison diagrams that the values of the simulated results are not consistent with the values of the monitoring results, and even the deviation are large and the data is not linearly correlated. However, the simulation data of the output concentration of CALPUFF is similar to that of the value of actual monitoring point, so the output of the model is considered to be reliable. This is similar to the findings of Zhang Dan's conclusion who used the CALPUFF model to simulate the visibility level in Chongqing. The results show that the CALPUFF air quality model can more directly simulate the distribution of pollutant concentration in the atmosphere[9].

3.2. Spatial distribution simulation analysis

3.2.1. The effects of diffusion simulation results are affected by the weather.

In this paper, the influence of weather field on pollutant dispersion was analyzed during the period from March 1st to March 8th in 2016.

From the figure 6 can be seen clearly, in March 1st to March 8th between the simulation of wind speed, the study period nearly 20 meters from the ground up to 7.18m/s, the southwest wind and the northeast wind was the main wind direction, the most popular west south. Due to the distribution of the emission source is mainly in the direction of the wind, therefore, the diffusion of pollutants in the direction has the most obvious, in the prevailing wind direction, the artillery academy and the Ermao of the two receiving points are of greater value. $\text{PM}_{10}$ distribution characteristics in March showed the spread to the northeast. The concentration of pollutants in the West and South was low, and the concentration in the East and North was high.

3.2.2. Analysis of influence of terrain elevation on diffusion result.

The city of Shenyang is located in the southwest corner of the whole Shenyang area. Compared with other counties and cities, the development of the transportation industry is relatively fast, and the pollution problems encountered are also serious. The whole area of Shenyang is dominated by plain or hilly terrain, which is relatively flat, and the trend of topography is low in east and west, with a height range of 18 to 270 meters. Combined with the research period of pollutants concentration size, accumulation of pollutants is easy to form in the region gathered, the terrain is unfavorable to contaminant transport, so that urban $\text{PM}_{10}$ particles within that time value is larger than the surrounding in other regions. The whole area is flat, and the pollutants in the surrounding cities will gather locally and be affected by the diffusion effect of the urban agglomeration.

3.3. Analysis of comprehensive factor simulation

Select the simulation results in the evening of March 1, 2016 at 0:00 and 21:00 night simulation results as an example(As shown in Figure 7):

The distribution of smoke plume at 0:00 is irregular and sporadic, and the distribution of this pollution state is mainly due to the different values of the initial emission concentration values of different emission sources. The main point source emission is located in the city of shenyang city, so the initial value is relatively high. The main emission enterprises in urban areas are mainly thermal
power plants, engine enterprises, ceramics enterprises and biotechnology, among them, thermal power generation mainly pollutes more than 50%.

Figure 7. Diffusion space view.

In order to better combine meteorological conditions, boundary field conditions, terrain elevation and other problems, select the same day at night 21 points concentration distribution of the situation to be analyzed, so that to analyze the factors that affect the simulation results.

In the simulation time for March 21, 2016, 21:00, the ground air direction to the southwest wind direction, because there is high pressure atmosphere, so the pollutants in Shenyang with the wind to
the northeast direction of the proliferation, leading to the monitoring point in the artillery academy value is relatively higher than other monitoring points. In the follow-up movement phase of the puff, direction had a tendency to spread eastward, considering the factors to remove the weather situation also involving the impact of geostrophic bias force. The concentration value of 21 o'clock on the evening of March 1st was larger than the concentration value of 0:00 am, due to March is the heating period of the northeastern region, coal and other large amounts of fuel burning resulting in larger particles in the night business, the phenomenon that factory of waste discharge was larger than the daytime.

4. Conclusions
The original wind field that generated by the WRF meteorological field was refined by the CALMET process, the result show that the southwestern and northerly winds appear more frequently during the simulation period. The concentration of the extraction points has a large value, which located in the downwind direction of the 11 monitoring points. From the land elevation document can be drawn: the southeast corner of the terrain is relatively high is not conducive to the proliferation of pollutants in the direction, and the whole territory of Shenyang relatively flat, resulting in wind speed, wind direction, pressure, temperature, the pollutants of surrounding cities and counties were easier to gather in the urban areas, resulting in urban concentration is too large. Combined with space layout and the concentration of sewage space distribution can be seen that most of the emission concentration of larger enterprise are located in or around Shenyang city, considering the influence of urban heat island effect and the inversion phenomenon, lead to atmosphere is stable and go against pollutant diffusion, easily lead to such as PM$_{10}$ substances over the city gathered, and make a fog haze weather.

Acknowledgment
The research supported by Liaoning province education department foundation (Item no.L2015405) and Doctor startup foundation in Shenyang Aerospace University (Item no.16YB17).

References
[1] Sheng Z 2017 Study on air pollution treatment in environmental engineering [J] Jiangxi building materials 11 288+290.
[2] Elbir T 2004 A GIS based decision support system for estimation, visualization and analysis of air pollution for large Turkish cities [J] Atmospheric Environment 38 4509-4517
[3] Tartakovsky D, Stern E, David M. Broday 2016 Comparison of dry deposition estimates of AERMOD and CALPUFF from area sources in flat terrain [J] Atmospheric Environment 10 430-432
[4] Elbir T, Mangir N, Kara M, et al.2010 Development of a GIS-based decision support system for urban air quality management in the city of Istanbul [J] Atmospheric Environment 44 441-454
[5] GB13271-2014 emission standard for boiler air pollutants [S] Environmental Protection Bureau 2014
[6] HJ/T 179-2005, technical specification for flue gas desulfurization in thermal power plant, lime water / lime gypsum method [S] National Environmental Protection Bureau 2005
[7] Zhong R, Haitao M, et al. 2011 Application of CALPUFF in Atmospheric Prediction and Environmental Capacity Accounting [J] Environmental Science and Technology 34(06) 201-205
[8] "CALPUFF model of technical methods and applications" Introduction [J] Environmental Impact Assessment 2016 38 (04) 4
[9] Dan Z, Zhen Z, Chongzhi Z 2013 CALPUFF model is used to simulate the visibility level of the main city of Chongqing [J] Ecology and Environment 35 (1) 9-11