Proceedings of the 3rd International Conference on Green Energy, Environment and Sustainable Development (GEESD2022), X. Zhang et al. (Eds.)

doi:10.3233/ATDE220297

A Review of PM2.5 in China—From the Qualitative and Quantitative Perspectives

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Abstract. According to the environmental bulletin in recent years, PM2.5 has been one of the primary pollutants of air pollution in China. And researches about PM2.5 in source analysis, composition, physical and chemical properties, prediction and other aspects have been studied. In order to better figure out the current research status of PM2.5 in China, this paper analyzes these related studies from the qualitative and quantitative aspects. From the qualitative aspect, the paper analyzes the composition and source of PM2.5. From the quantitative aspect, the paper describes the prediction method of PM2.5 concentration from two aspects, one is based on ground observation stations, the other is based on satellite data. Whether from a qualitative or quantitative perspective, the research on PM2.5 is still very necessary. The control of air pollution has a long way to go, and continuous research and practice are still required.

Keywords. PM2.5, composition, source analysis, prediction model

1. Introduction

Air pollution prevention and control is an important part of ecological environment protection in China, and it has been deepened with the evolution of major environmental problems in the process of social and economic development. From the 1970s to the early 1990s, total suspended particles (TSP, with a particle size of less than 100 microns) were mainly treated. In 1996, PM10 was included in the "Ambient Air Quality Standard (GB3095-1996)". PM2.5 was included in the new version of "Ambient Air Quality Standards (GB3095-2012)" until 2012. At present, China has done a lot of work in air pollution control and air quality management and achieved remarkable results, as shown in Figure 1, the proportion of PM2.5 as the main pollutant is continuously decreasing. But the pollution situation is still severe, and heavy pollution and serious pollution still occur. PM2.5 is harmful to human health [1-3], so it has always been the focus of the public and become one of the hot issues of the society. This paper will discuss the existing research about PM2.5 in China from both qualitative and quantitative perspectives.

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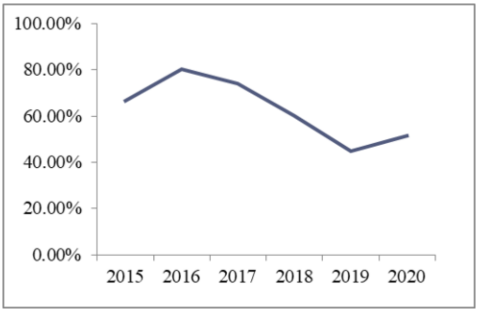

Figure 1. The proportion of PM2.5 as the main pollutant.

2. Composition of PM2.5

2.1. Water-Soluble Ions

Water-soluble ions are an important component of PM2.5, including SO_4^{2-}, NO_3^- and NH_4^+, in addition to a small amount of Cl^-, K^+, Mg^{2+}, Ca^{2+}, F^-, NO_2^- and other components [4-8]. NH_4^+, NO_3^-, SO_4^{2-} (called SNA) are the most important inorganic water-soluble ions in fine particles, SNA are a secondary pollutant generated from gaseous precursors SO_2, NO_x and NH_3 through homogeneous or heterogeneous reactions, and usually exist in the form of $(NH_4)_2SO_4$, NH_4HSO_4, H_2SO_4, NH_4NO_3 in the atmosphere [6]. These soluble components generally account for 20% to 50% of the mass of PM2.5. NH_4^+ mainly comes from the transformation of NH_3 produced in animal husbandry, agricultural fertilization and the degradation of organic matter. The formation of SO_4^{2-} is due to the burning of fossil fuels, which is higher in winter and lower in summer. NO_3^- comes from the conversion of its gaseous precursor nitrogen oxides. The nitrogen oxides in cities mainly comes from the emissions of motor vehicles, but industrial emissions, agricultural fertilizers also will cause the increase of NO_3^- [4, 9].

2.2. Carbon-Containing Components

Carbon-containing components are another important chemical component of PM2.5, accounting for 20-60% of the PM2.5 [10], which have an impact on atmospheric visibility [11], earth's Radiation Balance, and human health [12]. Carbon-containing components include organic carbon (OC), elemental carbon (EC), and carbonate carbon (CC). OC also contains a large amount of organic matter, such as aliphatic compounds, aromatic compounds, and organic acids. EC is also not elemental carbon in the simple sense, but a complex mixture, including pure carbon, graphitic carbon and other black non-volatile organic substances (such as tar, coke). CC includes sodium carbonate, potassium carbonate, magnesium carbonate and calcium carbonate and so on, which are ignored because of small content in PM2.5. The carbon components of PM2.5 mainly are from coal combustion, motor vehicle exhaust emissions and biomass combustion.

2.3. Inorganic Components

There are also a variety of metal elements and non-metal elements in PM2.5, containing Sodium (Na), Magnesium (Mg), Aluminum (Al), Copper (Cu), Sulfur (S), Boron (P), Chlorine (Cl), Potassium (K), Calcium (Ca), Nickel (Ni), Bromine (Br), Manganese (Mn), Zinc (Zn), Lead (Pb), Cadmium (Cd), Chromium (Cr), Antimony (Sb) and other nearly 40 species [13-17]. These elements are all primary particles, which are divided into natural sources (wind sand and volcanic eruptions) and anthropogenic sources. Metal elements contribute very little to the mass of PM2.5, usually less than 1% [18, 19]. Studies have shown that they not only have significant effects on particulate matter redox activity and oxidation potential [20, 21], but are also closely related to morbidity and mortality [22, 23].

3. Source Analysis of PM2.5

3.1. Source Analysis of PM2.5 Based on Air Quality Model

- **Industrial emission.** Metallurgy, building materials, petrochemicals and other key industries are the focus of regional industrial pollution prevention and control. The primary pollutant emissions of PM2.5 from industrial sources accounted for 60% of the total regional emissions. The primary emissions of PM2.5 in several key industries of iron and steel, coking, cement, glass and petrochemical accounted for 50% of the total emissions from industrial sources. During the heating period from 2016 to 2017, the contribution of industrial sources to PM2.5 was 25.3%-35.7% [24].

- **The usage of bulk coal for heating fuel.** In recent years, the conversion of coal to gas and coal to electricity has reduced the amount of scattered coal used, which directly affects the emission of air pollutants, especially SO_2 and primary PM2.5. Preliminary estimations show that in 2017 and 2018, the primary PM2.5 emission reductions are 23% and 34% under the measure. Moreover, the pollutant emission per unit of coal combustion is more than 15 times that of the power plant.

- **Mobile source pollution.** The number of mobile sources in China is numerous. From 2013 to 2018, car ownership increased by about 75 million. From 2009 to 2018, the number of motor vehicles in Beijing increased from 4.019 million to 6.084 million. Source analysis of fine particulate matter in Beijing's atmosphere in 2016 showed that the contribution rate of motor vehicle emissions reached 37.6% [25]; the source analysis results in 2018 showed that local emissions contributed 2/3, of which mobile sources accounted for 45% of local emissions. According to the latest source analysis results in 2020, local emissions are 60%, and mobile sources account for 46% of these 60%.

- **Dust.** Dust sources are divided into four categories: road dust, construction dust, soil dust and yard dust. Roads and construction are the main sources of fugitive dust in cities, and they can account for more than 80% of total fugitive dust emissions. The source analysis results of urban particulate matter for many years also show that although fugitive dust has been controlled to a certain extent, its contribution to PM2.5 concentration is still 15%-25%.

- **Catering fume.** The compositions of catering fumes are complex, including polycyclic aromatic hydrocarbons (PAHs), benzopyrenes, aldehydes and ketones, benzene series, heterocyclic amines and other harmful components. Studies have shown that most of the soot particulate matter emitted by catering is fine particulate matter. Taking the street as a unit, it is calculated that the PM2.5 emission intensity is 0.47 t/km-1.42 t/km^2 [26]. The latest analysis of PM2.5 sources released by Beijing in 2018 shows that catering sources contributed about 4%, while Guangzhou was about 6%.

3.2. Source Analysis of PM2.5 Based on Backward Trajectory Model

The characteristics of regional pollution are obviously one of the main characteristics of air pollution in China. The regional pollution is spatially manifested as the regional distribution of major cities with excessive pollution, and temporally manifested as the regional synchronization of heavy pollution processes. Cross-regional transportation is affected by terrain, meteorology and other conditions, and the transportation distance scales are different, ranging from within 100 meters to regional, countries.

Backward trajectory models are often used to identify possible external sources of particulate matter. In addition, methods such as Potential Source Contribution Factor (PSCF) and Concentration Weighted Trajectory (CWT) [27, 28] are used to identify potential sources. Li [29] used TrajStat and combined global data assimilation data to study the potential source areas that affected the concentration of particulate matter in Beijing from 2005 to 2016. In 2017, the regional transmission in Beijing accounted for 1/3, and the regional transmission contributed more than 50% when heavy pollution occurred; in 2020, the regional transmission accounted for 40%, mainly the southeast and southwest transmission channels. When heavy pollution occurs, the proportion of regional transmission is 64%. Figure 2 are results of the backward trajectory clustering, PSCF and CWT in Zhengzhou [30].

4. Quantitative Analysis of PM2.5

4.1. Prediction of PM2.5

There are two types of PM2.5 prediction models in Table 1: Mechanism models and Non-mechanism models. Mechanism models are mainly numerical prediction models [31]. Numerical models use various meteorological data and emission source data to simulate the formation of pollutants through the diffusion of atmospheric pollutants and the physical and chemical processes of substances, such as CAMQ [32], WRF-Chem [33], NAQPMS [34] etcetera. However, it is necessary to establish a relatively complete emission source inventory, meteorological field, and related models of physical and chemical changes involved in the process of pollutant diffusion.

Non-mechanical models include statistical models and machine learning models. Statistical models commonly used include multiple linear regression model [35], gray prediction model GM [36], ARIMA model [37]. With the development of machine learning, many scholars have also begun to apply machine learning methods to the prediction of PM2.5. We can divide these models into simple model and mixed models. Simple models only involve one of machine learning models, such as SVR [38], RF [39], BPNN [31], LSTM [40], etc. The mixed models are KNN-LSTM [41], LSTM-SVR [42], ARIMA-SVR [43], MRMR-HK-SVM [44], PCA-OS-ELM [45], etc. In the non-mechanism model, the variables used to predict PM2.5 have the following categories: pollutant data from monitoring stations; historical PM2.5 data; meteorological data; combination of pollutant data and meteorological factors, and maybe add other data such as boundary layer height and visibility. Compared with the mechanism model, the non-mechanism model requires relatively less data, does not involve the pollutant boundary field and the meteorological boundary field. The forecast model is simpler. Compared with statistical models, machine learning is more suitable for predicting PM2.5, and it can better deal with nonlinear problems. Because there are many factors affecting PM2.5 concentration, linear models may be difficult to describe clearly.

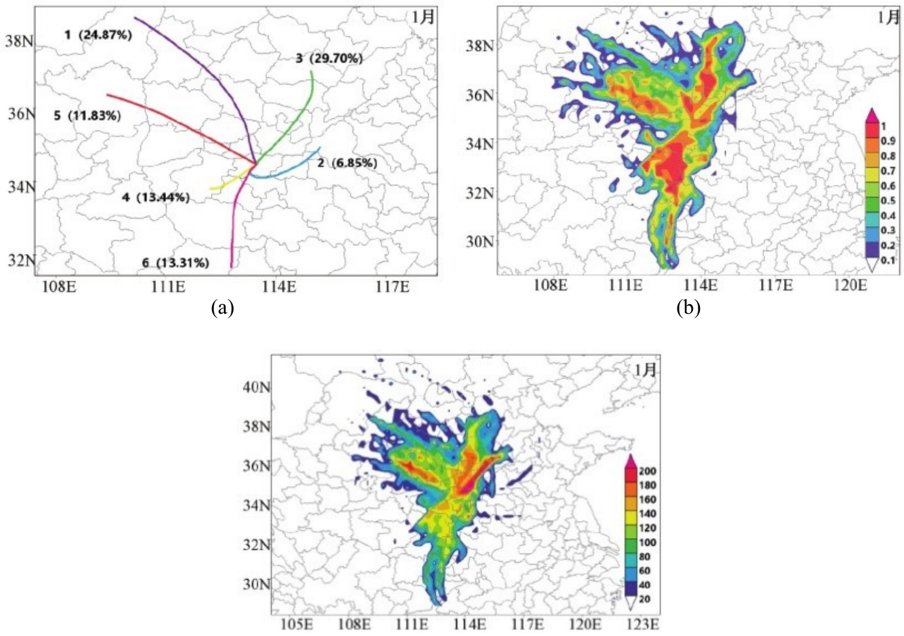

Figure 2. (a) Backward trajectory clustering; (b) PSCF; (c) CWT.

4.2. Estimation of PM2.5 Concentration Based on Remote Sensing Data

Aerosols are composed particles of solid and liquid particles suspended in the atmosphere. Many scholars have begun to use satellite data to discuss the estimation of atmospheric particulate matter concentration, which provide new ideas for the prevention and control of air pollution. Lots of studies have shown that there is a certain correlation between AOD and atmospheric particle concentration [46-48]. In order to make up for limitation of spatial distribution of ground-based monitoring stations, the estimation of PM2.5 by means of satellite remote sensing technology has become a research hotspot. There are four main methods to retrieve ground PM2.5 concentration based on satellite remote sensing AOD data in Table 2: Model scale factor method [49], Semi-empirical formula method, Statistical model method and Machine learning method [50].

Table 1. Comparison between mechanism models and non-mechanism models.

			Type	Advantage	Disadvantage
Mechanism model			CAMQ; WRF-Chem; CAMx; NAQPMS	Mature technology and relatively accurate results; suitable for a big scale	Low accuracy at small scale
Non-mechanism model	Statistical model		GM; ARIMA; GAM	Less data required, simpler model than mechanism model; Suitable for small regions	The complex mechanism process of PM2.5 Prediction is ignored.
	Machine learning model	Simple model	SVR; RF; LSTM; BP		
		Mixed model	KNN-LSTM; LSTM-SVR; ARIMA-SVR; MRMR-HK-SVM; PCA-OS-ELM		

The scale factor method was first proposed by Liu [51]. Liu used the chemical transport model of atmospheric pollution (CTM) to simulate the scale factor of AOD and PM2.5, and then used the scale factor to multiply the AOD obtained by satellite remote sensing. The advantage is that PM2.5 concentration can be simulated and calculated to obtain the particulate pollution situation in regions without PM2.5 monitoring sites. However, the method relies on the results of the model, and its parameters need to input accurate source list. Otherwise the accuracy of the model will be affected.

The type and vertical distribution of aerosols affect particle scattering characteristics and lead to differences in scattering extinction, but the physical mechanism is relatively complex. Therefore, scholars have studied the semi-empirical formula for estimating PM2.5 from the characteristics of different aerosol types and hygroscopic effects to estimate ground PM2.5 [52-53]. This method takes into account the physical mechanism between AOD and PM2.5, and the inversion results are also better than the scale factor method [54]. But there are also some shortcomings. The relationship between AOD and PM2.5 is very complex and cannot be expressed by a complete formula. The parameters in the formula are difficult to obtain under the existing conditions, and it is difficult to apply it in practice.

The statistical model can be divided into simple linear regression and advanced statistical models. One is to establish a simple linear regression model between AOD and PM2.5 [55]. The second is the advanced statistical model [56-58]. In addition to AOT, factors such as meteorological data, boundary layer height and location are added to the model. The advanced statistical model not only expands research scope, but also improves the accuracy of PM2.5 retrieval from satellite remote sensing, making it more widely used. The method requires a large amount of data to support the fitting and verification of the model, and the limitation is that it is only used in the area of PM2.5 monitoring sites. The more factors introduced into the formula, the higher the complexity among parameters. On this basis, the expression of nonlinear relationship may not be optimal.

With the development of machine learning, scholars have gradually introduced these methods into estimation of PM2.5. There are backward neural network and artificial neural network [58], as well as SVM, RF, etc. The precision of them is higher than others. But the results obtained by machine learning methods cannot be materialized or explained in mathematical language, and it is currently impossible to improve them according to the relevant materialized mechanisms. The "black box" nature hinders researchers to understand model results [50]. However, for massive samples, self-supervision and training of machine learning have greater advantage, and the estimation accuracy is higher. There is no difference between machine learning result and statistical models result, but it will appear overfitting phenomenon when the number of samples is small.

Table 2. Comparison of different methods.

		Advantage	**Disadvantage**
Scale factor method		Not rely on ground-based PM2.5 observation data	Parameters cannot be updated; low precision; high cost
Semi-empirical method		Better precision than scale factor method	Part of parameters are difficult to obtain
Statistical method	Simple linear regression model	Simple model	Not consider the influence of the physical mechanism between AOD and PM2.5 on the estimation accuracy
	Advanced Statistical Models	Higher precision by introducing more parameters	
Machine learning method		Considering the nonlinear relationship between model parameters; high estimation accuracy	Results cannot be explained in materialized mechanisms or mathematical language

5. Conclusions

This paper mainly expounds the existing research papers on PM2.5 from two perspectives qualitative and quantitative. Due to space limitations, the relevant elaboration on PM2.5 may not be comprehensive enough. In terms of qualitative aspects, the composition, sources and hazards of PM2.5 are expanded. The composition of PM2.5 is mainly divided into three categories, water-soluble ions, carbon-containing components and inorganic elements. The main sources are industrial emissions, mobile sources, fugitive dust, coal use and catering sources. From a quantitative point of view, it is mainly in describing the prediction and estimation of PM2.5. The prediction of PM2.5 is based on ground monitoring data, and different models are used for prediction; the other is based on remote sensing data, which is also estimated using a variety of models. Both have their own advantages and disadvantages. The former can make accurate predictions on a small scale, but it cannot be applied on a large scale. The latter just makes up for this. Qualitative analysis and quantitative analysis are indispensable in the research of PM2.5. The two complement each other and provide directions and ideas for the governance of PM2.5.

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