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Regional-level prediction model with advection PDE model and fine particulate matter ($PM_{2.5}$) concentration data

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Abstract

Real-time and geo-tagged data on $PM_{2.5}$ enable researchers to model and predict the trends of air pollution effectively. On the basis of network and clustering, a specific advection partial differential equation (PDE) model is proposed to forecast the spatial-temporal dynamics of $PM_{2.5}$ concentration at large scale of city-cluster. The proposed PDE model incorporates the effects of advection, local emission and dispersion. The prediction is performed in real-time with varying model parameters for assessing the current situation. Good simulation results not only demonstrate the proposed PDE has good prediction ability, but also show that the model can quantify the advection and local effects for the air pollution of each city-cluster to some extent. Moreover, the methodology can be extended to other types of air pollution provided that data are available.

Keywords: air pollution, network and clustering, advection-PDE model, temporal-spatial prediction, advection effects

(Some figures may appear in colour only in the online journal)

1. Introduction

$PM_{2.5}$, a kind of atmospheric particulate matter, has a diameter of less than 2.5 μm and thus has been confirmed to be associated with many respiratory diseases and even causes damage to the nervous system [1]. Accurate assessment of ambient $PM_{2.5}$ concentration is essential for environmental and public health risk analysis, which has aroused unprecedented concern worldwide. Although many ground-based air monitoring stations have been established to provide hourly $PM_{2.5}$ concentration data in China, measurements based on points are non-continuous. Moreover, we require accurate prediction results to help human and governments make decisions.

Considering the nonlinear characteristics of $PM_{2.5}$ variation, high-quality prediction has been a popular problem and has remained a challenge for scientists and researchers in different fields. *Satellite sensing techniques* demonstrate advantages of spatially seamless and long-term coverage; thus, they have been extensively used to predict $PM_{2.5}$ in recent years [2]. Recently, an *ordinary differential equation model* has been proposed to describe the temporal variations of air quality index in a local province [3]. This model can describe the time dynamics of air pollution but is only adaptable for a local spatial position and cannot describe transboundary effects. *Statistical model:* Many more history data have been accumulated given the gradually expending air monitoring networks. This provides the convenience for applying statistical model to make predictions. Statistical models often have high computational efficiency and simple modeling principles, but they need long history data. *Machine learning* [1, 4, 5] is a kind of interdisciplinary integrated learning method involving statistics, data science, and computing. This kind of method demonstrates strengths in handling complex nonlinear relationships between various predictors and the final prediction results; It is easy to operate and with high accuracy. However, the disadvantage of this method is also prominent, that is the main mechanism behind the prediction can not be provided [4]. For instance, the reasons for the predictions' high accuracy can

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not be effectively explained, which is insufficient to convince a key decision makers [6]. *Chemical transport model* (Mathematically, it is depicted by *PDE system*) mainly predicts from the view of the formation mechanism of $PM_{2.5}$. This method can predict $PM_{2.5}$ concentrations without historical observations but requires knowledge of the temporal dynamic processes of the emission quantities of various pollutants [7]. Besides, the relative PDE system, for instance of nonlinear time-dependent reaction-convection-diffusion (transport) system, consists numerous partial differential equations (PDEs) by nonlinear coupling many chemical species, successfully describing the spatial interactions between individuals of the system. However, such problems are frequently accompanied by large-scale, computationally challenging problems [8, 9].

Actually, to overcome large-scale computational complexity and make high-accuracy spatial-temporal prediction meanwhile, we have attempted to build pollution-transport network, then cluster cities (through clustering, the spatial locations can be dimensional reduced into several city-clusters), and finally provide a specific diffusion PDE model to describe the spatial-temporal dynamics of the single chemical species, $PM_{2.5}$ [10]. However, if the goal is to explore the air pollution transport in a large spatial scale, only the term 'diffusion' is insufficient, and the term 'advection' must be incorporated.

The present work aims to explore the air pollution transport in a large spatial scale (between city-regions) and further make prediction. Therefore, we incorporate the 'advection' term. Specifically, based on network and clustering for 189 cities of China, we incorporate the advection term and a local emission (or dispersion) term to build a specific PDE model for modeling and predicting $PM_{2.5}$ spatial-temporal dynamics globally at the city-region level. Moreover, this model can quantify the advection and local effects for the air pollution of each city-cluster.

Though advection PDE models have been extensively used to describe air pollution transport in many previous work, the background of pollution problem always give rise to large-scale calculations just as the illustration above. Therefore, it is the first try to combine network, clustering (through clustering, the spatial locations can be dimensional reduced into several city-clusters) and then a specific advection PDE to make temporal-spatial prediction of air pollution globally at city-region level. For the specific model, large-scale computation is not needed. Meanwhile, simulation results demonstrate that the model not only has good prediction ability but also can provides policy insights to some extent.

2. Model

In this section, we aim to develop a specific PDE model to describe the temporal-spatial transport of air pollution at the city-cluster level. We take 189 cities of China for example, as the data is so.

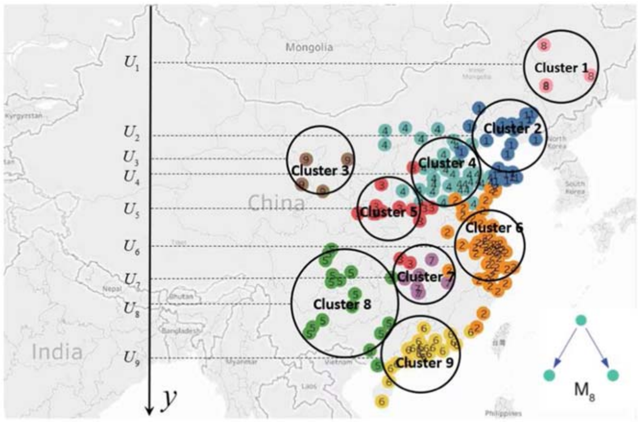

Figure 1. City-clusters obtained by using M_8-motif spectral clustering algorithm [13].

2.1. Network building and clustering

As we research the regional transport of $PM_{2.5}$, first we divide all the 189 cities into different city-clusters; then it is convenient to provide a specific PDE to describe the spatial-temporal transport of $PM_{2.5}$ between these city-regions. In reality, it is more meaningful to do research on city-clusters than single cities, as air pollution is transboundary, clustering cites provides the standard for defining the scopes and priorities for joint prevention and control of air pollution regions [11]. The obtained city-clusters can be regard as the basic regions of joint-control for air pollution [11]. Below we sketch how to build $PM_{2.5}$ transport network of 189 cities in China, then cluster cities, and finally build the connection with PDE model by projecting these city-clusters into Euclidean Space.

The sketch is that: (1) *Network building*: We use network to describe the complex air transport system. That is, regard each city as a network node. The presence of $PM_{2.5}$ directional transport between cities A and B determines whether a directional weighted edge exists from Node A to Node B in the network (It is the integrated result based on real observation data about wind direction, wind speed, and geographic distance.); thus, a city network with 189 cities is built. Mathematically, it is described by a weighed adjacency matrix. (2) *Clustering cities*: We cluster network on the basis of higher-order connectivity patterns. Here we choose subgraph M_8 (M_8 reflects the movements of $PM_{2.5}$ from source to target) as the basic building block of the network, method of higher-order spectral clustering [12] is used to obtain 9 city-clusters. In figure 1, nodes (representing cities) with the same color are located in the same cluster. More specific process refers to our previous work [13]. (3) *Projecting city-clusters into Euclidean space*: Because wind is the main factor that influences air transport, and China experiences monsoon winds, thereby indicating that most wind directions are from south to north or from north to south. Simply, we project Clusters 1–9 located from north to south in the map of China onto the y-axis of the Cartesian coordinates. Thus, each city-region has its relative spatial location y.

On the basis of all the preparatory work above, a specific one-dimensional PDE model is provided to describe the regional transport of air pollution below.

2.2. PDE model building

Let $u(y, t)$ represent the concentration of $PM_{2.5}$ at location y at a given time t. The changing rate of $u(y, t)$ mainly depends on two processes: (i) regional transport due to the wind effect and it contributes most air pollution as mentioned in [14–16]; (ii) local emission and dispersion. Therefore, the dynamics of $PM_{2.5}$ is depicted by equation (1)

$$\begin{aligned} \frac{\partial u(y,t)}{\partial t} &= -g(y)\frac{\partial u(y,t)}{\partial y} \\ &\quad + r(t)u(y,t)\left(h(y) - \frac{u(y,t)}{K}\right), \\ u(y,1) &= \phi(y), \quad l < y < L, \\ u(1,t) &= \psi(t), \quad t \geqslant 1, \end{aligned} \tag{1}$$

- $-g(y)\frac{\partial u(y,t)}{\partial y}$ describes the regional transport (transboundary pollution) of $PM_{2.5}$ between different city-clusters; this term has been used for describing the spatial movement of chemicals given wind effects [17] and is called an advection term.
  1. $g(y)$ is the mean velocity at location y. In this study, we assume that $g(y)$ has the form of $g(y) = b_5 + \mathrm{e}^{-b_6(y-b_7)}$, $b_6 \geqslant 0$, $b_7 \geqslant 0$. This form shows a tendency of wind speed to decrease from north to south.
  2. $\frac{\partial u(y,t)}{\partial y}$ can be positive or negative, which describes the integrated effect of air flow on air pollution of location y at time t. For example, when $\frac{\partial u(y,t)}{\partial y} < 0$, the integrated effect of air flow increases the pollution concentration of location y at time t, as $-g(y)\frac{\partial u(y,t)}{\partial y} > 0$ is valid.

     It is called the integrated effect of the air-flow due to the following reasons: for each city-cluster at location y, (i) all the cities have different wind directions and wind speeds. Even for the same city, wind varies during the whole day. Therefore, it is the integrated effect of wind from different cities over the whole day; (ii) when $-g(y)\frac{\partial u(y,t)}{\partial y} > 0$ is valid, we can not identify whether the high-pollution winds blow in or the low-pollution winds blow away. However, it is certain that the whole effects of air-flow lift the pollution concentration of the city-cluster at location y.
- $r(t)u(y,t)\left(h(y) - \frac{u(y,t)}{K}\right)$ presents the local pollution process in a local city-cluster, which includes local emission (the primary aerosol, such as road dust, vehicle exhaust, industrial emissions and the secondary aerosol) and dispersion in a local cluster.
  1. The function $r(t) > 0$ denotes the intrinsic growth rate or dissipate rate of $PM_{2.5}$ of the cluster at location y and time t, regulated by meteorological conditions. $PM_{2.5}$ may be produced as secondary aerosol due to the external temperature, pressure, etc; or $PM_{2.5}$ may be dissipated, such as rain. Therefore, we denote $r(t)$ as $r(t) = b_2 + \mathrm{e}^{-b_3(t-b_4)^2}$ and it may increase or decrease along with time t. Here, parameters b_2, b_3, b_4 are determined by using real data.
  2. The location function $h(y)$ represents the heterogeneity of $PM_{2.5}$ due to spatial location. Different city-clusters represent different regions in China (as in figure 1). Different levels of economy and population from various regions lead to essentially distinct $PM_{2.5}$ emission amounts and dissipate rates. In this study, $h(y)$ is built through a cubic spline interpolation, thereby satisfying $h(y_i) \equiv h_i$, $i = 1, 2, \ldots, 9$, where y_i represents the spatial location of city-cluster i. $h(x)$ is determined by the latest $PM_{2.5}$ concentration data.
  3. The function $-\frac{u(y,t)}{K}$ describes that air pollution does not increase indefinitely over time, and a maximum carrying capacity K of the environment exists. This part extensively exists in the logistic model, thus modeling the population dynamics, where the rate of reproduction is proportional to existing population and amount of available resources [18]; this part has also been used to describe information diffusion in online social networks, which consist of the maximum possible density of influenced users at a given distance [19].
- $u(1,t) = \psi(t)$, $t > 1$ is the boundary condition at location $y = 1$. $\psi(t)$ can be constructed from the history data of $PM_{2.5}$ at location $y = 1$ through cubic spline interpolation.
- $u(y,1) = \phi(y)$ is an initial $PM_{2.5}$ concentration function, that can be constructed from the history data of $PM_{2.5}$ through the cubic spline interpolation.

Standard meteorological models, such as the Unified Danish Eulerian model [8], describes air pollution by a system of PDEs; the temporal dynamic processes of the emission quantities of various chemical species must validate the PDEs; such problems may consist of a multiple equations, thereby leading to large-scale, computationally challenging problems [9]. Model (1), which we proposed in the present study, concentrates on globally describing the temporal-spatial characters of specific air pollution for different city-clusters, thereby only requiring data from specific chemical species, such as case of $PM_{2.5}$ in this study.

In addition, advection-diffusion equation is frequently used to describe air pollution in the atmosphere [20], in which air pollution can be advected by an underlying bulk flow field and diffusion occurs without any bulk flow. To explore the air pollution transport among different city-clusters, we do not consider the diffusion effects in Model (1) given the large spatial scale.

3. Data and PDE-based prediction

The basic mathematical properties of PDE Model (1), such as existence, uniqueness, and positivity of the solution of the model, can be established from the standard theorems for parabolic PDEs [21]. Below we use real data to build PDE model with time-varying parameters and perform prediction in real-time.

3.1. Data

In the present study, we explore the temporal-spatial transport characteristics and further make the temporal-spatial prediction for $PM_{2.5}$ in China at a large scale of different city-clusters. Two groups of daily data are needed: one is for the network building and then clustering cities; the other is for PDE prediction.

To build network and then obtain the 9 city-clusters illustrated in section 2, data from 1 January, 2015 to 30 June, 2015 are used in this work (Here we remark it as Data-set 1). Actually, we can use data in other time period to build network as well, as long as the time interval of Data-set 1 is earlier than the period we want to make prediction for pollution. For example, if we want to predict the pollution in February of 2016, we can first build the network based on the data in January of 2016. Specifically, the following kinds of data are needed for network building: (i) $PM_{2.5}$ monthly average concentration from China National Environmental Monitoring; (ii) Latitude and longtitude of 189 cities from Google Earth; (iii) Wind speed and wind direction data is from the China Meteorological Administration. More specific data description and preparatory work can refer our previous work of [13].

To make prediction using the provided PDE model, parameters involving in the PDE should first be determined. Therefore, sectional data of different days regarding $PM_{2.5}$ concentrations must be obtained. Here, we only require the data of $PM_{2.5}$ concentration during the latest several days to build the specific models (it refers to determine the parameters in the PDE) and predict the concentration on the following day. We focus on the research period from 1 January, 2016, to 5 July, 2016 to valid our PDE model in the perspective of prediction (Here we remark it as Data-set 2). This data set covers heavily polluted winter and ordinary days. A total of 189 priority pollution-monitoring cities in Mainland China, covering all 34 provincial-level regions of China, are all included. The most polluted cities and the cities of interest, such as Beijing and Shanghai, are involved.

We handle Data-set 2 through the following steps. First we compute the average $PM_{2.5}$ daily concentration of each cluster every day by averaging the daily $PM_{2.5}$ concentration of all the cities included in this cluster. Thus, we obtain the daily average $PM_{2.5}$ concentration of each cluster. Second, the $PM_{2.5}$ concentrations of each city-cluster are normalized to a discrete level value of 1, 2,…, or 6, in accordance with the 'Ambient Air Quality Standards' (GB3095-1996) of China, where $PM_{2.5}$ concentrations are divided into 0–35, 36–75, 76–115, 116–150, 151–250, and $\geqslant 250\,\mu$g. The different concentration ranges use Levels 1–6, which correspond to excellent, good, lightly polluted, moderately polluted, heavily polluted, and severely polluted air quality. Linear scaling makes a concentration value to a specific range, which ensures that large value input attributes do not overwhelm small value inputs, thereby helping decrease prediction errors.

3.2. PDE-based prediction

The $PM_{2.5}$ concentration of every city-cluster is influenced by environmental policies, economics, population movement, and weather variations. Thus, the parameter values of the model must vary with time but with the same underlying structure model (1). In this study, the parameters in the PDE model are real-time, as determined using real $PM_{2.5}$ concentration data.

The whole prediction procedure is as follows. To predict the concentration of Day 4, we use the training data set of Days 1, 2, and 3. First, we interpolate the discrete data of Day 1 for constructing the initial function $\phi(x)$ and interpolate the discrete data of Cluster 1 at Days 1, 2, and 3 for constructing the boundary function $\psi(x)$. Second, we use the data of Days 2 and 3 to train the parameters of the PDE model. Finally, we solve this PDE model with initial function $\phi(x)$ and boundary function $\psi(x)$ to predict the $PM_{2.5}$ concentration of Day 4. By applying the same procedure, we use the training data of continuous 3 d to predict the $PM_{2.5}$ concentration for the following day. For instance, we use Days 1–3, 2–4, and 3–5 as training data to obtain the model parameters, then predict Days 4–6, correspondingly.

In performing prediction, the parameters must be estimated. Essentially, these parameters comprise a list of THE multi-parameter inverse problem of a parabolic equation. Hybrid methods combine the advantages of local and global methods: global optimization is first used to explore the parameter space to locate the starting points for further local optimization [22]. In the present study, we combine a tensor train global optimization approach [23] and Nelder–Mead simplex local optimization method [24] to train the PDE parameters, where the Nelder–Mead simplex method corresponds to the fminsearch function in MATLAB.

After each determining the model parameters, we combine the characteristic method and fourth-order Runge–Kutta algorithm to compute the PDE for one-step forward prediction numerically.

4. Modeling results

4.1. Model prediction accuracy

In this study, we apply relative accuracy (RA) $1-\frac{|u_{\text{real}}-u_{\text{predict}}|}{u_{\text{real}}}$ and absolute increment accuracy (AIA) $1-\frac{|u_{\text{real}}-u_{\text{predict}}|}{5}$ to measure the prediction accuracy. In these domains, u_{real} represents the actual $PM_{2.5}$ concentration at each spatial location of every data collection time point, and u_{predict} is the predicted $PM_{2.5}$ concentration based on Model (1). The accuracy definition of RA is a rule that measures the accuracy of $PM_{2.5}$ concentration value, whereas AIA is a rule that measures the prediction accuracy in the view of the $PM_{2.5}$ concentration level. Typically, we disregard the specific concentration of $PM_{2.5}$, such as 30 or 33. We care more about that whether $PM_{2.5}$ is good, slightly polluted, medium polluted, or heavily polluted. Therefore, we also apply AIA to measure the prediction accuracy, which has been used in our previous work [10].

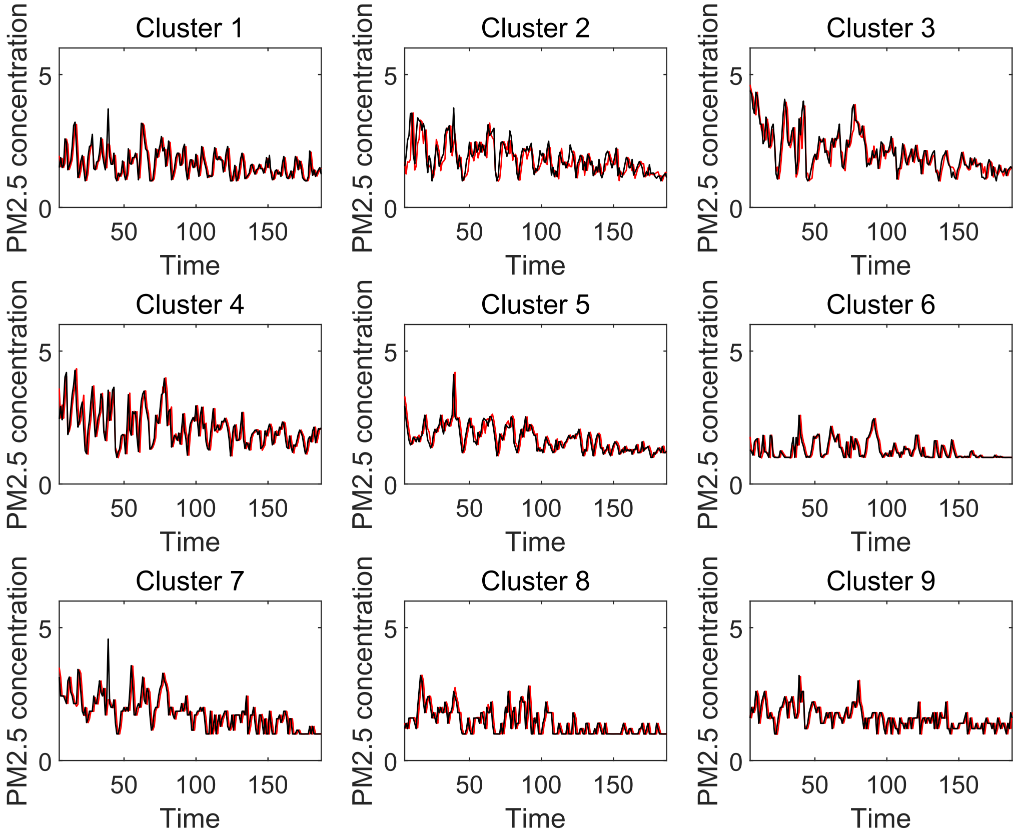

Figure 2. Daily PM2.5 concentration level from 5 January, 2016, to 6 July, 2016. The black lines represent the real data and red lines represent prediction results based on Model (1).

Figure 2 illustrates the prediction results in Regions 1–9 every day from 5 January, 2016, to 5 July, 2016. Evidently, a consistent trend can be observed between the predicted data of Model (1) (represented by red lines) and real observations (represented by black lines). Figure 3 demonstrates the prediction accuracy in each city-cluster from 5 January, 2016, to 7 July, 2016. Clearly, the RA and the AIA of approximately all the regions during the prediction period nearly exceed 0.8 and 0.9, respectively. Table 1 summarizes the average relative accuracies and average AIA of each city-cluster forecasted based on Model (1). In table 1, our proposed PDE-based prediction model exhibits a strong prediction ability with average prediction accuracy exceeding 0.8 and 0.9 in accordance with our accuracy measures.

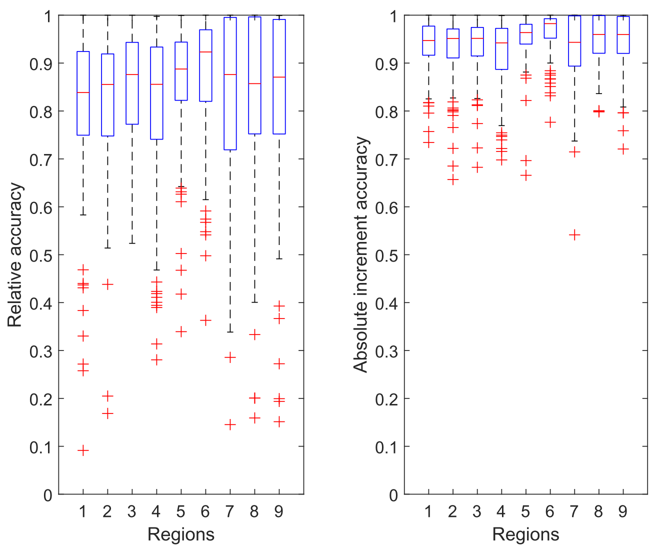

Figure 3. The prediction accuracy in each city-cluster from 5 January, 2016, to 7 July, 2016. Here relative accuracy is the conventional definition as $1-\frac{|u_{\mathrm{real}}-u_{\mathrm{predict}}|}{u_{\mathrm{real}}}$ and absolute increment accuracy is defined as $1-\frac{|u_{\mathrm{real}}-u_{\mathrm{predict}}|}{5}$; u_{real} is the actual $PM_{2.5}$ concentration at each spatial location of every data collection time point; u_{predict} is the predicted $PM_{2.5}$ concentration based on Model (1).

4.2. Model description ability

In section 2, the changing rate of $PM_{2.5}$ concentration (marked by $u(y,\, t)$) mainly depends on local pollution rate (marked by $r(t)u(y,\, t)\left(h(y)-\frac{u(y,t)}{K}\right)$, which is positive) and regional transport rate (transboundary pollution)through advection (marked by $-g(y)\frac{\partial u(y,t)}{\partial y}$, which may be positive or negative). During our research period of 182 d from 5 January, 2016, to 7 July, 2016, we accumulate all the local emission effects of each city-cluster by accumulating the values of $r(t)u(y,\, t)\left(h(y)-\frac{u(y,t)}{K}\right)$ in each region. Meanwhile, we accumulate all the advection positive (negative) effects and the relative number of days of each city-cluster. The statistical results are listed in table 2. For instance of 35.31(89), it denotes 89 d out of 182 d, in which advection has increased local $PM_{2.5}$ concentrations, and the total effect

Table 1. Average prediction accuracy of nine city-clusters, where MRA means average relative accuracy and MAIA means average absolute increment accuracy.

	$R1$	$R2$	$R3$	$R4$	$R5$	$R6$	$R7$	$R8$	$R9$
MRA	0.81	0.82	0.85	0.81	0.86	0.88	0.82	0.84	0.83
MAIA	0.94	0.93	0.94	0.92	0.95	0.97	0.94	0.95	0.95

Table 2. The advection and local emission effects for the nine city-regions among the 182 d from 5 January 2016, to 7 July, 2016. Values outside parentheses are the accumulated effects and values in the parentheses are the relative number of days resulting to these effects. For instance of 35.31(89), it denotes 89 d out of 182 d, in which advection has increased local $PM_{2.5}$ concentrations, and the total effect index is 35.31.

Advection effect	$R1$	$R2$	$R3$	$R4$	$R5$	$R6$	$R7$	$R8$	$R9$
$-g(y)\frac{\partial u}{\partial y} > 0$	35.31 (89)	34.03 (91)	34.25 (90)	40.24 (80)	23.00 (98)	19.42 (122)	31.78 (114)	25.17 (130)	28.39 (109)
$-g(y)\frac{\partial u}{\partial y} < 0$	−27.9 (93)	−25.1 (91)	−26.2 (92)	−37.2 (102)	−17.4 (84)	−13.9 (60)	−27.3 (68)	−19.5 (52)	−21.5 (73)
Local effect	$R1$	$R2$	$R3$	$R4$	$R5$	$R6$	$R7$	$R8$	$R9$
$r(t)u\left(h(y) - \frac{u}{K}\right)$	7.20 (182)	8.50 (182)	5.08 (182)	2.69 (182)	3.87 (182)	5.19 (182)	2.36 (182)	5.45 (182)	6.90 (182)

index is 35.31. −27.9(93) indicates 93 days out of 182 d, in which advection decreases the local $PM_{2.5}$ concentrations, and the total negative effects index is 27.9. In table 2, regional transport through advection contributes most of the air pollution in each city-region. In [15], the air quality of Shanghai is largely influenced by the air masses from the north, east, and west, thus accounting for 44.8%, 30.4%, and 24.8% of all the air masses, respectively. In [16], the contribution of the regional transport to $PM_{2.5}$ is estimated in Lingcheng on the North China Plain; in addition, the $PM_{2.5}$ concentration from the regional transport contributes 31.6% of the $PM_{2.5}$ concentrations, with only 15.4% from the local emissions.

5. Discussion and conclusion

In the context of air pollution, many models have been used to study the prediction problem. In this study, on the basis of network and clustering, a specific advection PDE model is proposed to characterize and predict the daily $PM_{2.5}$ concentration at city-region level. The integration of network, clustering, and advection PDE model to regionally explore air pollution is the first attempt. This attempt avoid the large-scale computation problem of the traditional PDE system. From the numerical simulations, combining PDE models with real data can provide substantial information on the $PM_{2.5}$ spatial-temporal dynamics. Our study is $PM_{2.5}$-specific, as the data is so. Nevertheless, the methodology can be extended to other types of air pollution provided that data are available.

Given that regional transport brings most of the air pollution for a city-cluster as mentioned in [14–16], we incorporate advection to describe the effects of air-flow in our mechanistic PDE model. Although advection term has been extensively used in a system of PDEs to describe the dynamic processes of multiple chemical species, we aim to globally describe the temporal-spatial characteristics of specific air pollution. Through advection, the air pollution from advection effects is tractable. Our simulation results demonstrate that regional transport through advection contributes most of air pollution in each city-region. This finding is consistent with the research from the atmosphere field [15, 16]. In addition, based on our scaling data in section 3.1, we obtain the quantifiable advection and local effects for each city-cluster. We can compare the relative values of both effects to measure them from the regional transport and local emission or dissipation perspective. However, these values, as well as whether these values describe the real phenomenon, require assistance and must be further confirmed by meteorologists. Moreover, we aim to explore the air pollution transport between different city-clusters and ignore the diffusion effects in Model (1) given the large spatial scale.

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