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Mathematical modeling of Fog-Haze evolution

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ABSTRACT

Under the global warming, the significant changes in atmospheric water cycle lead to drying in arid region, which is strengthening the effect of aerosol on Fog-Haze generation and accelerating the emergence of infectious diseases. However, the production process of the Fog-Haze is lack of quantitative description based on atmospheric water cycle. In this paper, we modeled the process of Fog-Haze generation, evolution and disappearance fundamentally and theoretically. The budget functions for water vapor and aerosol were coupled by the physical and chemical interaction between water vapor and aerosol. The obtained results may provide new insights on the control of Fog-Haze and the related infectious diseases induced by Fog-Haze.

1. Introduction

In recent years, many areas, especially China, are suffering a serious impact of Fog-Haze [1–5]. It was reported that no more than one percent of the first 500 largest cities in China reached the air quality standards recommended by World Health Organization [3,6]. The main negative impact of haze on human being includes increasing mortality, chronic diseases exacerbate, respiratory system and worsen heart disease [1], reducing the reproductive ability and changing the structure of the body's immunity. It will also affect the formation of clouds and rainfall, lead to arid region becoming drier, wet zone getting wetter, climate-induced disasters.

Generally, Fog-Haze forces the spread of infectious diseases mainly in three ways: (1) As a result of the weakened Ultraviolet in the near-surface layer, the activity of infectious bacteria in the air is enhanced and infectious diseases are increased; (2) Hazardous substances carried by Fog-Haze damage human respiratory system and reduce human immunity to infectious diseases; (3) Haze particles as carriers of infectious bacteria, spread in the air, increased the probability of transmission through the transmission. Physical processes of the atmosphere decides the generation, Evolution and disappearance of Fog-Haze, through accumulating, transporting and exchanging atmospheric aerosol and water vapor [5]. Atmospheric moisture and condensation nuclei, that is aerosol, are generally the internal factors of the generation of Fog-Haze. There is a complex interaction between water vapor and aerosol. From the monomer to the storm cloud systems, due to the feedback of different scales, water vapor and the aerosol affecting the physical processes of atmosphere, especially the atmospheric water cycle process, through participation in the formation of clouds, fog and haze [7]. For example, condensation nuclei changes will significantly alter the storms of spatial-temporal distribution of precipitation, the frequency distribution of rainfall rate and the height of cloud base and top [8–10]. Air pollution causes an increase in the density of aerosol, and leads to more very small cloud droplets [7,11]. The anthropogenic pollutants emitted from vehicles and unfavorable meteorological conditions exerted a great influence on PM2.5 and black carbon loading and increased the cloud condensation [12]. The continuing role of aerosols leading to reduced precipitation [13] often induces a more stable atmosphere, which is more conducive to the accumulation of air pollutants and contributes to the formation of haze events [14]. Meanwhile, the haze layer will cause thermal diffusion, which occupy the sky lasting moisture, so that rain events decrease during dry season, but intensify during the rainy season [15]. In addition, the pollution of haze droplets may be related to droplet mean volume radius and may depend on the temperature and atmospheric humidity [16,17].

On the contrary, the atmospheric water cycle will also affect the production, Evolution and disappearance of haze. The relative humidity determined by atmospheric water vapor content affects the microstructure of haze, clouds and precipitation [18]. The moisture content tends to produce larger more rain clouds and precipitation in the form of clean air in the atmosphere [2,19], which reduces haze generation to a certain extent. In general, the efficiency

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of clearing wet aerosol particles is strongly influenced by the rainfall intensity and depends on the haze particle size [20]. The larger particles is the better rain washes [19]. On the other hand, increasing aerosol can in turn make the precipitation rate decrease [21], which is more conducive to the generation of haze. Aerosol particles mainly consist of biomass combustion, industrial emissions, mine dust, dust and so on. They will diffuse and transfer between adjacent area. The particulate ingredients were different in different regions [22–25]. The influence of water vapor on aerosols depended on the components of aerosol [26,27] and regional characteristics [28]. After complex chemical-physical interaction, such as oxidation, vapor phase nucleation, phase nucleation and growth processes [29–31], the original emission particles and water vapor generate secondary aerosol particles.

Projected changes in the water cycle over the next few decades show similar large-scale patterns to those towards the end of the century, but with smaller magnitude. Changes in the near-term, and at the regional scale will be strongly influenced by natural internal variability and may be affected by anthropogenic aerosol emissions [32].

It can be concluded from above that, water vapor and its condensation nuclei, that is atmospheric aerosol particle, play the leading roles in the formation of Fog-Haze. The circulating of atmospheric water vapor and aerosol particles timely control the dynamic distribution of regional water vapor and aerosol, which directly affects the formation, evolution and disappearance of Fog-Haze. Since global warming, the significant changes in atmospheric water cycle caused reducing precipitation and drying in arid region [33–35], which strengthen the effect of aerosol on haze generation [7,36]. However, the quantitative description and associated prediction mode for the production process of the haze based on water cycle is still unclear. In this paper, to reveal the mechanism of the interaction between atmospheric water vapor and condensation nuclei during atmospheric physical processes from the perspective of hydrological cycle, we model and simulate the process of Fog-Haze generation, evolution and disappearance fundamentally and theoretically.

2. Mathematical modeling of the generation, evolution and disappearing of Fog-Haze

2.1. The function of transformation between water vapor and aerosol

In the atmosphere, many secondary aerosol particles are produced from the complex interactions between any two of aerosol particles and water vapor. In this study, all processes of physical-chemical effects including oxidation, vapor and liquid phases nucleation, and growth, are defined as the material conversion. The related conversion equation is:

$$(j)a_{\Omega i} + (k)H_2O + (l)O_2 = h_{\Omega i}, \tag{1a}$$

where $a_{\Omega i}$ is the *i-th* aerosol particles; $h_{\Omega i}$ is the corresponding secondary aerosol particles; $(l)O_2$ is optional and only exists in the material oxidation reaction. For example, the interaction among SO_2, H_2O and O_3 can be represented as

$$3SO_2 + 3H_2O + O_3 = 3H_2SO_4 \tag{1b}$$

2.2. The budget functions for water vapor and aerosol

The factors of weather and climate conditions and human activities affecting on the generation of Fog-Haze are very complex. The factors of weather and climate conditions, such as evaporation, precipitation, wind, temperature and so on, and human factors like pollutant emissions, emission type and distribution, as well as physical and chemical reactions between different particles, may lead to changes of water vapor and aerosol concentration in the area. But no matter how change they do, their quality must comply with the law of conservation of matter. Therefore, the dynamic distribution of the water vapor and aerosols within the region and can be calculated and monitored by the balance equations.

We suppose that the atmospheric water vapor content in region Ω at time t is $W_\Omega(t)$, then

$$\frac{\partial W_\Omega(t)}{\partial t} + \frac{\partial[W_\Omega(t)u]}{\partial x} + \frac{\partial[W_\Omega(t)v]}{\partial y} = E_\Omega(t) - P_\Omega(t) + \beta_\Omega(t), \tag{2}$$

where x and y denote the longitude and latitude respectively; $\partial[W_\Omega(t)u]/\partial x$ and $\partial[W_\Omega(t)v]/\partial y$are the divergence term due to atmospheric movement; u and v are macroscopic horizontal velocities of water vapor and particles and mainly related with the meridianal and zonal wind speed; $E_\Omega(t)$ and $P_\Omega(t)$ are evaporation and precipitation respectively; $\beta_\Omega(t)$is the reaction diffusion term, it is namely the additional items generated from the random diffusion of water vapor and aerosols in the unit time and generating substance after material conversion. $\beta_\Omega(t)$ is expressed as:

$$\beta_\Omega(t) = d\left\{\frac{\partial^2 W_\Omega(t)}{\partial x^2} + \frac{\partial^2 W_\Omega(t)}{\partial y^2}\right\} - f_\Omega(t) \tag{3}$$

where $f_\Omega(t)$ is the reaction term obtained by the substance-conversion equation, d is the diffusion coefficient.

Similarly, we assume that there are n kinds of primary aerosol particles in region Ω and the content of the i-th particle at time t is $Q_{\Omega i}(t)$, then

$$\frac{\partial Q_{\Omega i}(t)}{\partial t} + \frac{\partial[Q_{\Omega i}(t)u_i]}{\partial x} + \frac{\partial[Q_{\Omega i}(t)v_i]}{\partial y} = A_{\Omega i}(t) + \alpha_{\Omega i}(t) \tag{4}$$

where $A_{\Omega i}(t)$is the quality of ith aerosol particle generated by natural or human emissions within the region per unit time at time t; $\partial[Q_{\Omega i}(t)u_i]/x$ and $\partial[Q_{\Omega i}(t)v_i]/\partial y$ are divergence term generated from the atmospheric motion; u_i and v_i are the macroscopic meridianal and zonal velocity of ith aerosol particle and are affected by the wind speed and physical properties of the particles; $\alpha_{\Omega i}(t)$ is an additional item resulting in the physical-chemical reaction (material conversion), random diffusion and sedimentation and meets to

$$\alpha_{\Omega i}(t) = d_i\left\{\frac{\partial^2 Q_{\Omega i}(t)}{\partial x^2} + \frac{\partial^2 Q_{\Omega i}(t)}{\partial y^2}\right\} - f_{\Omega i}(t) - s_{\Omega i}(t) \tag{5}$$

where d_i is the diffusion coefficient; $f_{\Omega i}(t)$ is the reaction term, determined by the material conversion equation; $s_{\Omega i}(t)$ is the sedimentation item, aerosols will gradually settle and disappear when their gravity or density is large enough.

2.3. Coupling the matter transformation into the budget equation

Since atmospheric aerosols are composed of variety particles, they have different physical and chemical properties, such as particle size, water-soluble and so on. These different physical and chemical properties of aerosols determine the way and speed they combined with water vapor are not the same. This correspondingly leads to different secondary aerosol particles systems and different influences of climate change on the process of their generating, developing and disappearing. Therefore, a substance conversion-mass balance coupled model need to establish to characterize the formation of aerosol particles system. Here, we add the material conversion equation as coupling terms to balance equations.

Fig. 1 is the framework of the substance converted-balance equation coupled model. Firstly, the amount of n kinds of aerosol

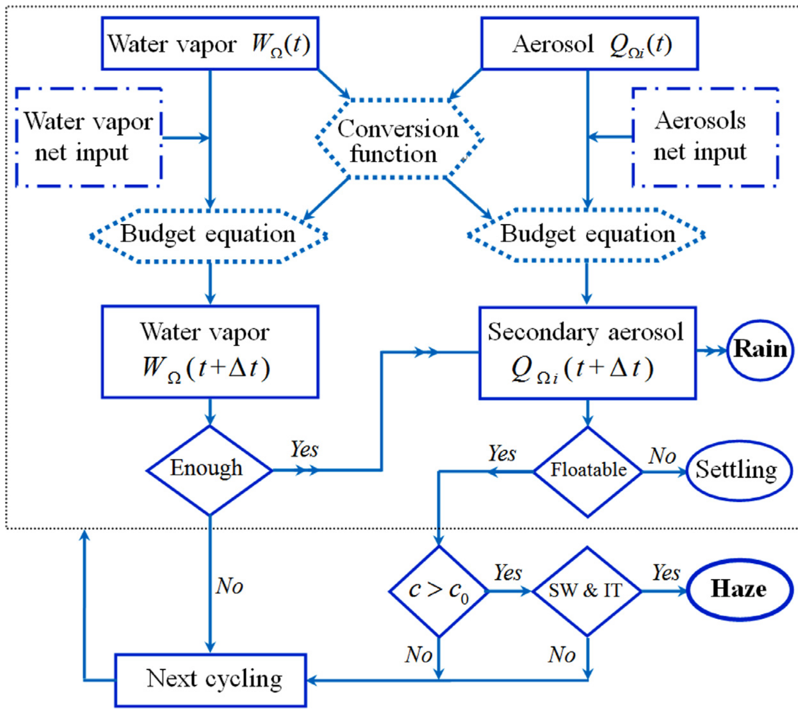

Fig. 1. The framework of matter conversion–balance equation coupled model (SW: Static wind; IT: inversion temperature; Enough: $r_H \geq 90\%$, r_H represents the air relative humidity).

particles and water vapor within region Ω at time t are calculated respectively according to the initial conditions, and the water vapor and aerosols net input are computed based on zero-flux boundary condition which means that no external input is imposed from outside; Secondly, we estimate the secondary aerosol particles generated from material conversion equation and give the additional items of balance equation at time $t + \Delta t$; Thirdly, we couple the additional items to the equilibrium equation to calculate the amount of water vapor and aerosol at $t + \Delta t$ moment; Then we estimate the settling velocity of various secondary particles. If the settling speed is less than a certain value, this kind of particle can be considered as suspended particulate matter and we will statistics its concentration; Finally, we diagnose whether the Fog-Haze occur according to the concentration and static wind and inversion air temperature.

In this process, the total mass of all the suspended aerosol particles at time $t + \Delta t$ also meet the balance equation

$$H_\Omega(t+\Delta t) = H_\Omega(t) + \sum_{i=1}^{n} \Delta H_{\Omega i}(t) - \sum_{i=1}^{n} H^{w}_{\Omega i}(t+\Delta t) - \sum_{i=1}^{n} H^{T}_{\Omega i}(t+\Delta t), \quad (6)$$

where $H^{w}_{\Omega i}(t+\Delta t)$is the additional items when the secondary aerosol particles are blown off by too heavy horizontal wind; $H^{T}_{\Omega i}(t+\Delta t)$ is the additional items considering the thermal uplift. Given static wind and inversion air temperature, both of them are zero, then

$$H_\Omega(t+\Delta t) = H_\Omega(t) + \sum_{i=1}^{n} \Delta H_{\Omega i}(t). \quad (7)$$

Therefore, under the conditions of calm wind and inversion temperature, scarce water vapor tends to promote the suspended aerosol particles to increase and accelerate the generation and Evolution of Fog-Haze. On the contrary, abundant ($r_H \geq 90\%$, $r_H$represents the air relative humidity) moisture being supported to the aerosol particles enlarges the precipitated particles and makes it to grow up to raindrops falling to the ground as precipitation. Once this situation forms, the haze will gradually dissipate.

3. Conclusion and discussion

In this paper, we present a mathematical model on the evolution of Fog-Haze mainly with respect to atmospheric water vapor content and aerosol particles. Under the framework of our study, one can reveal the intrinsic mechanisms on the formation of Fog-Haze. Our work is a start point on the understanding of Fog-Haze and may provide some useful measures on Fog-Haze control.

It should be noted that Fog-Haze may promote the transmission of infectious diseases, such as cholera [37,38], brucellosis [39,40], hemorrhagic fever with renal syndrome [41] and so on [42]. In this sense, when taking control measures for disease, we need to consider the effects of Fog-Haze. Analyzes of the evolution of Fog-Haze require that data to be highly precise, both in space and time, and also need complex analysis to describe them in detail. When these requirements are met, the approach appears quite useful for targeting Fog-Haze control in space and time. Such collaborations, if successful, would stimulate the further development of this emerging research area.

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