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Modelling multi-component aerosol transport problems by the efficient splitting characteristic method

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HIGHLIGHTS

- Modelling multicomponent aerosol transport problems in atmospheric environment
- A splitting characteristic FDM for general multicomponent aerosol transport models
- The developed algorithm is robust and efficient for large-scale applications

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ABSTRACT

In this paper, a splitting characteristic method is developed for solving general multi-component aerosol transports in atmosphere, which can efficiently compute the aerosol transports by using large time step sizes. The proposed characteristic finite difference method (C-FDM) can solve the multi-component aerosol distributions in high dimensional domains over large ranges of concentrations and for different aerosol types. The C-FDM is first tested to compute the moving of a Gaussian concentration hump. Comparing with the Runge-Kutta method (RKM), our C-FDM can use very large time step sizes. Using $\Delta t = 0.1$, the accuracy of our C-FDM is 10^{-4}, but the RKM only gets the accuracy of 10^{-2} using a small $\Delta t = 0.01$ and the accuracy of 10^{-3} even using a much smaller $\Delta t = 0.002$. A simulation of sulfate transport in a varying wind field is then carried out by the splitting C-FDM, where the sulfate pollution is numerically showed expanding along the wind direction and the effects of the different time step sizes and different wind speeds are analyzed. Further, a realistic multi-component aerosol transport over an area in northeastern United States is studied. Concentrations of $PM_{2.5}$ sulfate, ammonium, nitrate are high in the urban area, and low in the marine area, while sea salts of sodium and chloride mainly exist in the marine area. The normalized mean bias and the normalized mean error of the predicted $PM_{2.5}$ concentrations are −6.5% and 24.1% compared to the observed data measured at monitor stations. The time series of numerical aerosol concentration distribution show that the strong winds can move the aerosol concentration peaks horizontally for a long distance, such as from the urban area to the rural area and from the marine area to the urban and rural area. Moreover, we also show the numerical time duration patterns of the aerosol concentration distributions due to the affections of the turbulence and the deposition removal. The developed splitting C-FDM algorithm can be applied to model spatial multi-component aerosol transport problems in large domains in atmosphere.

1. Introduction

Recently, it has been recognized that aerosols play an important role in global climate warming and change as well as air pollution. Atmospheric aerosols are solid, liquid, or mixed-phase fine particles suspended in air. They are one of most important constituents of atmosphere and have significant impact on environment and human health. Aerosols have a direct radiative forcing by scattering and absorbing solar and infrared radiation in atmosphere and have indirect forcing by changing cloud precipitation patterns which leads to the change of global circulation systems that constitute the Earth's

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climate. Aerosols are also associated to the formation of haze, dust, dust storm, acid fogs, acid rains and related air pollution (Friedlander, 2000; Lee et al., 2015). Small aerosol particles can be inhaled into the human body and induce adverse health effects. In these processes, the physical states and distribution variation of the multi-component aerosols are of great significance. It is important to numerically study the aerosol processes and aerosol concentration distributions in environmental prediction and air quality control.

Spatial aerosol transport model is a complex multi-component system of partial differential equations, which involves spatial transport and dispersion, emission, deposition, aerosol dynamic processes of condensation/evaporation and coagulation, and aerosol chemical process. Some efforts have been made in the computation of the aerosol concentration distributions in various regions. Odman and Russell (1991) studied the URM model and the UAM-AIM and applied them in the aerosol simulations in the southern California. Gaydos et al. (2007) and Mebust et al. (2003) studied the PMCAMx and the Models-3/CMAQ and carried out simulations over eastern United States. Grell et al. (2005) developed the WRF/Chem model and simulated the aerosol concentration distributions over the eastern United States and contiguous areas. There were further studies over areas in Europe (Nopmongcol et al., 2012), east Asia region (Koo et al., 2008) and Yangtze River Delta region in China (Wang et al., 2012). There are also some research focusing on small scale aerosol studies, for instance, the investigation of the interaction between the aerosol formation and turbulence (Barbaro et al., 2015; Lee et al., 2014) and the study on the land surface/atmosphere interactions (Nemitz and Sutton, 2004). The aerosol simulations are usually performed over a long period and cover a large region which is discreted into a huge number of grids. However, very small time steps have to be used in simulations in order to ensure the stability of the numerical schemes for aerosol transport solution, which brings a huge cost of computation and leads to the limitation of application. With the increase of large scale simulation in applications, there is a growing need to develop efficient numerical methods that can ensure high-accurate multi-component aerosol simulation results by using large time step sizes for decreasing computational cost.

In this paper, we consider general multi-component aerosol transport problems in atmosphere that involve the spatial transport and dispersion, emission, deposition, aerosol dynamics, and aerosol chemical process and develop the efficient characteristic finite difference method (C-FDM) to solve the transport and dispersion process in the spatial aerosol dynamic system by combining with the operator splitting technique to deal with emission, deposition, aerosol dynamic and chemical processes. The methods of characteristics were first proposed in (Douglas and Russell, 1982) to solve single dimensional convection-diffusion problems and were further developed for high-dimensional convection diffusion problems in (Arbogast and Huang, 2010; Celia et al., 1990; Liang et al., 2007; Pokrajac and Lazic, 2002), etc. The methods can reduce the truncation errors in time and allow to use large time sizes in computation. In numerical experiments, we first test our C-FDM to simulate the moving of a Gaussian concentration shape in two dimensions, where the high accuracy is obtained by our C-FDM using a large time step size compared to those used in the RKM. Second, we investigate a transport of the sulfate pollution in a varying wind field with different mesh grids, different time step sizes and with different wind speeds. Results show that the highest aerosol concentration is located near the emission area, and the sulfate plume transports along the wind direction. Further, we study a realistic multi-component aerosol transport simulation over an area in northeastern United States. The predicted $PM_{2.5}$ concentrations are compared to measured data taken at United States Environment Protection Agency (EPA) monitor stations. The analysis of the aerosol components distributions for an urban, a rural and a marine area shows that the urban area has the highest $PM_{2.5}$ concentration among the three areas, while the marine area has the lowest $PM_{2.5}$ concentration. The time series of numerical aerosol concentration distribution show that the strong winds can move the aerosol concentration peaks horizontally for a long distance. Finally, we numerically study the aerosol optical properties and the affections of the turbulence and deposition. The urban area has a low single scattering albedo (SSA) of 0.87 at the wavelength of 600 nm due to the large concentration of sulfate and other absorbing aerosols, while the SSA of rural and marine areas are 0.917 and 0.986. The predictions reveal that nitrate concentrations always peak at the nighttime when temperature is low, since the nitric acid only transferred to the aerosol phase after reaction with other species under lower temperatures as computed by ISORROPIA for the aerosol themodynamics (Nenes et al., 1998). When we simulate the turbulence using the MYJ (Mellor-Yamada-Janjic) PBL (planetary boundary layer) scheme (Mellor and Yamada, 1982) instead of YSU (Yonsei University) scheme (Hong et al., 2006), the predicted temperature has a mean decrease of 1.09 °C, which leads to a higher nitrite concentration. Effects of deposition on aerosol concentrations are studied and numerical results show that deposition plays an important role in the removal of aerosols, especially in the removal of aerosols with large sizes. The developed splitting C-FDM algorithm can be applied for modelling spatial aerosol distributions using large time steps and for simulating the large scale predictions of multi-component aerosols in atmosphere.

The paper is organized as follows. Section 2 introduces the general multi-component aerosol transport model. The splitting characteristic finite difference method is proposed in Section 3. Numerical simulations are given in Section 4. Finally, conclusions are given in Section 5.

2. The general multi-component aerosol transport model

The aerosol distributions in atmosphere vary considerably in space, time and particle size. The variability of the aerosol concentrations is determined by several complicated physical and chemical processes: transport and dispersion (including the advection in large scale and turbulence in small scale), emission, deposition, aerosol dynamics and aerosol chemistry. The general multi-component aerosol transport model is (Seinfeld and Pandis, 2012; Wexler et al., 1994):

$$\frac{\partial c_l}{\partial t} = -\mathbf{U}\cdot\nabla c_l + \nabla\cdot(K\nabla c_l) + E_{l,Emis}(\vec{x},v,t) + \Lambda_{l,Dep}c_l + \mathscr{L}_{l,Aero} + (\vec{c}) + \mathscr{R}_{l,Chem}(\vec{c}), \qquad l = 1,2,\cdots,s, \tag{2.1}$$

$$c_l(\vec{x},v) = c_l^{IN}(\vec{x},v), \quad \vec{x}\in\Gamma_{IN}, \tag{2.2}$$