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THE TIME SECOND-ORDER CHARACTERISTIC FEM FOR NONLINEAR MULTICOMPONENT AEROSOL DYNAMIC EQUATIONS IN ENVIRONMENT

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Abstract. An efficient time second-order characteristic finite element method for solving the nonlinear multi-component aerosol dynamic equations is developed. While a highly accurate characteristic method is used to treat the advection multi-component condensation/evaporation process, a time high-order extrapolation along the characteristics is applied to approximate the nonlinear multi-component coagulation terms. The scheme is of second order accuracy in time for the multi-component problems. We study the theoretical analysis and obtain the time second-order error estimate of the scheme. Numerical experiments are further given to confirm the theoretical results. The dynamic behaviours of multi-component aerosol distributions are also simulated for the multi-component aerosol problems of aerosol water, black carbon and sulfate components with different tri-modal log-normal initial distributions.

Key words. Multi-component aerosol dynamic equations, condensation/evaporation, nonlinear coagulation, characteristic method, characteristic extrapolation, error estimate.

1. Introduction

Global climate change and warming in atmosphere have been widely recognized. As one of most important constituents, aerosols are minutes particles suspended in atmosphere, which play an important role in climate change, atmospheric chemistry, and air pollution issues including visibility reduction and adverse human health effects. The research on the multi-component aerosol dynamics is of great importance, which can provide a better understanding of the distribution of aerosol particles in atmospheric environment and can further help to predict and protect the atmospheric environment. Modeling the composition and size distributions of atmospheric aerosols is very important as they determine the optical properties of particles, and moreover, the aerosol composition influences the ability of particles to act as cloud condensation nuclei or ice nuclei.

The evolution of the size distribution of aerosols is governed by the nonlinear aerosol dynamic equation, which describes the impacts of several processes such as condensation, coagulation, emission, and deposition, etc. Some numerical methods were developed, including sectional method [3, 7], moment method [5, 12], modal method [1, 16], stochastic approach [4], finite element method [13], etc. The sectional method is simple but usually leads to numerical diffusion when treating condensation/evaporation [7]. The modal method has high efficiency but has less physical representation of aerosol distributions and less accuracy. The moment method is not suitable for the simulation of multi-modal distributions. The drawback of the stochastic method is that it can not get a satisfied accuracy. Recently,

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[8] proposed a splitting wavelet method for solving the spatial aerosol dynamic equations on time, particle size and vertical coordinates. Due to the condensation advection and the nonlinear coagulation, modelling accurately and efficiently the sharp distributions of aerosols still is a challenge work in computation of the multi-component aerosol dynamic equations.

The multi-component aerosol dynamic equations are described as follows. Let $q_i(m,t)$ be the mass concentration distribution for species i of aerosol particles having total particle mass in the range m to $m + \mathrm{d}m$ at time t. N_c is the total number of chemical species. The change rate of the total mass of a particle of mass m caused by condensation/evaporation is denoted by

$$I(m,t) = \sum_{i=1}^{N_c} I_i(m,t), \tag{1}$$

where $I_i = \frac{\mathrm{d}m_i}{\mathrm{d}t}$, m_i is the mass of species i in a particle of total mass m. The normalized condensation/evaporation rate of species i is

$$H_i(m,t) = \frac{1}{m}\frac{\mathrm{d}m_i}{\mathrm{d}t}, \tag{2}$$

and the total condensation/evaporation rate is

$$H(m,t) = \sum_{i=1}^{N_c} \frac{1}{m}\frac{\mathrm{d}m_i}{\mathrm{d}t} = \sum_{i=1}^{N_c} H_i(m,t). \tag{3}$$

The multi-component aerosol general dynamic equations are ([11, 14, 15])

$$\begin{aligned} \frac{\partial q_i(m,t)}{\partial t} &= H_i(m,t)\sum_{j=1}^{N_c} q_j(m,t) - \frac{\partial(mq_iH)}{\partial m} \\ &+ \int_{M_{\min}}^{m-M_{\min}} \beta(m,m-m')q_i(m,t)\frac{\sum_{j=1}^{N_c} q_j(m-m',t)}{m-m'}\mathrm{d}m' \\ &- q_i(m,t)\int_{M_{\min}}^{M_{\max}} \beta(m,m')\frac{\sum_{j=1}^{N_c} q_j(m',t)}{m'}\mathrm{d}m', \ \ t\in(0,T], m\in\Omega, \end{aligned} \tag{4}$$

$$q_i(M_{min},t) = 0, \quad t\in[0,T], \tag{5}$$

$$q_i(m,0) = q_i^0(m), \quad m\in\Omega, \quad i = 1,2,\cdots,N_c, \tag{6}$$

where $t > 0$ is the time, and $T > 0$ is the time period; the finite mass interval $\Omega = [M_{\min}, M_{\max}]$ where $M_{\min} > 0$ is the minimal mass and $M_{\max} > 0$ is a finite maximal mass. $\beta(m,m')$ is the coagulation kernel function. Eq. (4) forms a system of N_c nonlinear integral-differential equations on time and particle mass.

In this paper, we develop and analyze a time second-order characteristic finite element method (FEM) for solving the multi-component aerosol dynamic equations by taking the advantage of characteristic technique, which can solve the problems accurately and efficiently. In our method, we first transfer the time derivative term and the advection-condensation term into the global derivative term along the characteristics and then approximate it by the difference operator along the characteristic curve, where more accurate solution can be obtained. For treating the nonlinear coagulation term, by using two previous time level values, we propose to use a time second-order extrapolation, i.e. a combination of previous two level values of coagulation terms along the characteristics. The developed characteristic FEM scheme is of second-order accuracy in time and can provide efficiently high accuracy solutions when using large time step sizes. The study of the method has been examined for