The theoretical analysis of TEMOM model for particle population balance equation due to Brownian coagulation

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Aerosol particles are increasingly recognized as one of the most common unhealthy components of air pollution. Researchers have already shown that there is a strong correlation between mortality and particle size, with specific reference from nanoparticles to fine particles (Jacobson et al. 2005). The evolution of nanoparticles is controlled by the population balance equation (PBE), which is a nonlinear partial differential equation (Friedlander, 2000). The PBE is capable of describing the particle evolution under all kinds of processes (i.e., advection, diffusion, coagulation, nucleation, surface growth, etc.). However, it is computationally demanding to directly solve the PBE because of its dependence on the particle volume. For the relative simplicity of implementation and low computational cost (Pratsinis, 1988), the moment method has become a powerful tool for investigating aerosol microphysical processes in most cases.

Recently, Yu et al. (2008) have presented a new, moment-based numerical approach termed as the Taylor-series expansion method of moment (TEMOM) to solve the coagulation equation. In this model, the moment equations are closed using a Taylor-series expansion technique. Through constructing a system of the first three order ordinary differential equations, the most important moments for describing the aerosol dynamics, namely, the particle number density, particle mass and geometric standard deviation, are obtained. This approach makes no prior assumption on the shape of the particle size distribution (PSD); therefore, this property of the TEMOM model makes it to be prior to the existing classical lognormal model (Yu et al., 2009; Xie et al., 2012).

In the present study, mainly as a methodological introduction, I would attempt to show the recent progresses in theoretical investigation of TEMOM model for Brownian coagulation. Based on the TEMOM model, an elegant asymptotic solution of PBE for Brownian coagulation has been obtained not only in the free molecule and continuum regime (Xie and Wang, 2013) but also in the transition regime (Xie, 2014), and the asymptotic results show that all moments at long times depend explicitly on time and particle first moment (i.e., particle mass concentration). Recently, the analytical solution of TEMOM model for particle coagulation in the free molecule and continuum regime has been obtained directly based on the Taylor series (Xie and He, 2013). All these works are powerful proof of the validity for the TEMOM model. Although the TEMOM models are not the original PBE equations, the solutions for them also provide the important information for PSD. Due to the analytical solution's natural property, it needs less computational cost, but provide the same accurate result as the numerical method. Therefore, this method is worthy getting more attention by aerosol modelers if they need to solve PBE equation in their works. To establish and improve the theoretical system of TEMOM model, Xie and He (2014) have clarified some fundamental problem, such as the uniqueness of the expansion, the effectiveness for the closuring fractional moments, the choice of the expansion point, the convergence of the analytical solutions, and the inverse problem, etc. but the accuracy of higher moment and error estimation are still remained to be solved.

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