THE TAYLOR-EXPANSION METHOD OF MOMENTS FOR THE PARTICLE SYSTEM WITH BIMODAL DISTRIBUTION

by

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Short paper
DOI: 10.2298/TSCI1305542L

This paper derives the multipoint Taylor expansion method of moments for the bimodal particle system. The collision effects are modeled by the internal and external coagulation terms. Simple theory and numerical tests are performed to prove the effect of the current model.

Key words: *bimodal, multi-point Taylor expansion, TEMOM, aerosol dynamics*

Introduction

As a typical aerosol system, a bimodal particle system attracts more and more attention [1], because it is often found in the urban on-road environment, which consists of both the nano particles emitted from vehicles and the background ones [2, 3]. Its diameter ranges 5 nm-2.5 μm. The variation in diameter will lead to the different dynamic regime of particles, which is less considered in the previous study.

Method of moments (MOM) is one of the most effective techniques to evaluate the evolution the aerosol system. There are typical three kinds of methods: pre-determined PSD [4], quadrature method of moment (QMOM) [5] and Taylor expansion method of moment (TEMOM) [6, 7]. Among all the existent MOM techniques, TEMOM utilizes the Taylor expansion to solve the closure problem of MOM [8], which is proved to be precise and computational cheap. However, TEMOM expands the collision term at a single point, *i. e*. the systematic average diameter, which will lead to error for bimodal system. The additional error may attribute to the large difference of diameters for the particle in different modes. For example, the average diameter may be 100 nm for a certain bimodal system with only two kinds of particles: 5 nm and 2.5 μm. TEMOM will expand at 100 nm for both modes, which produces extra error.

The current study focuses on the multipoint TEMOM to reduce such error. The expression is deduced and both theoretical and numerical tests are performed to evaluate the new model.

Theories

The bimodal particle size distribution (PSD) can be expressed as: $N(v, t) = N_i(v, t) + + N_j(v, t)$ [9]. Hence, the particle balance equation (PBE) [10] for each sub-PSD will be established [11]. Take moments of N_i and N_j in the volume space, the final moment equations for bimodal system can be expressed as:

$$\frac{\partial m_k^i}{\partial t} = C_k^{ii} + D_k^{ij} \tag{1}$$

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$$\frac{\partial m_k^j}{\partial t} = C_k^{ij} + E_k^{ij} \tag{2}$$

where $C^{ii}{}_k$ and $C^{jj}{}_k$ are the internal coagulation in the modes i and j, $D^{ij}{}_k$ and $E^{ij}{}_k$ – the external coagulation between the modes i and j. The exact expression can be written:

$$C_k^{ii} = \frac{1}{2}\int_0^\infty\int_0^\infty [(u+v)^k - u^k - v^k]\beta(u,v)N_i(u)N_i(v)\mathrm{d}u\mathrm{d}v \tag{3}$$

$$D_k^{ij} = -\int_0^\infty\int_0^\infty u^k \beta(u,v)N_i(u)N_j(v)\mathrm{d}u\mathrm{d}v \tag{4}$$

$$E_k^{ij} = \int_0^\infty\int_0^\infty [(u+v)^k - v^k]\beta(u,v)N_i(u)N_j(v)\mathrm{d}u\mathrm{d}v \tag{5}$$

In the expression of $C^{ii}{}_k$, $D^{ij}{}_k$, and $E^{ij}{}_k$, the collision kernel β means the collision possibility between particles with volume u and v, and its treatment is the key point of TEMOM. Re-write β as:

$$\beta(v_1, v_2) = B_1(v_1 + v_2)^{1/2}(v_1^{1/6}v_2^{-1/2} + 2v_1^{-1/6}v_2^{-1/6} + v_1^{-1/2}v_2^{1/6}) \tag{6}$$

Expand β at multipoint ($v_1 = u_1$, $v_2 = u_2$) using a Taylor expansion. Note that $C^{ii}{}_k$ and $C^{jj}{}_k$ are only related with N_i or N_j, the result from typical TEMOM can be directly used at u_1 or u_2) [12, 13]:

$$C_0^{ii} = \frac{-\sqrt{2}B_1}{5184u^{23/6}}(-214m_2^i m_0^i u^2 - 4388m_1^{i2}u^2 + 1424m_2^i m_1^i u + 6691m_0^{i2}u^4 - 65m_2^{i2} + 6920m_1^i m_0^i u^3)$$

$$C_1^{ii} = 0 \tag{7}$$

$$C_2^{ii} = \frac{-\sqrt{2}B_1}{2592u^{11/6}}(-6748m_1^{i2}u^2 + 701m_2^{i2} - 1034m_2^i m_0^i u^3 - 176m_1^i m_0^i u^3 - 3176m_2^i m_1^i u + 65m_0^{i2}u^4)$$

In eq. (7), m_k^i represents the k-th moment of PSD in mode i. For D_k^{ij} and E_k^{ij}, focus on the non-linear part $(v_1 + v_2)^{1/2}$ and neglect the terms higher than 3 order. If $u_{12} = u_1 + u_2$, $r = u_2/u_1$ is defined, the expansion can be written as:

$$(v_1 + v_2)^{1/2} \approx \frac{3}{8}\sqrt{u_{12}} + \frac{3}{4}\frac{v_1 + v_2}{\sqrt{u_{12}}} - \frac{1}{8}\frac{(v_1 + v_2)^2}{u_{12}^{3/2}} \tag{8}$$

Substitute eq. (8) into eqs. (4) and (5). Equations (4) and (5) can be converted into a formula without integration. At the same time, a lot of fractional moments will appear and the moment equations remain opening. The fractional moments can be approximated through the expansion of v^p (p is fraction) at u_1 or u_2:

$$m_p \approx \frac{u^{p-2}(p^2 - p)}{2}m_2 - u^{p-1}(p^2 - 2p)m_1 + \frac{u^p}{2}(p^2 - 3p + 2)m_0 \tag{9}$$

Make use of eq. (9), $D^{ij}{}_k$ and $E^{ij}{}_k$ can be expressed as a linear combination of $m^i{}_k$ and $m^j{}_k$. In these expressions, a_{mn}, b_{mn}, c_{mn}, d_{mn}, and e_{mn} are the coefficients related only with r and u_1. For context compactness, the exact expressions of them are not listed:

$$D_0 = -\frac{\sum a_{mn} m_m^i m_n^j}{2592 u_{12}^{3/2} u_1^{14/3} u_2^{14/3}},\ D_1 = -\frac{\sum b_{mn} m_m^i m_n^j}{2592 u_{12}^{3/2} u_1^{14/3} u_2^{8/3}},\ D_2 = -\frac{\sum c_{mn} m_m^i m_n^j}{41472 u_{12}^{3/2} u_1^{14/3} u_2^{2/3}},\ E_0 = 0,$$

$$E_1 = -\frac{\sum d_{mn} m_m^i m_n^j}{2592 u_{12}^{3/2} u_2^{14/3} u_1^{8/3}}, \qquad E_2 = -\frac{\sum e_{mn} m_m^i m_n^j}{41472 (u_{12})^{3/2} u_2^{14/3} u_1^{2/3}}$$

Validations and discussion

Both the theoretical and numerical tests are performed to verify our model. First of all, note that if $N_i = N_j = N/2$, eqs. (1) and (2) turn into two sets of moment equations with mono-modal distribution. If eq. (1) plus eq. (2) and set $m_k = m_k^i + m_k^j$, the full moment equations should be: $\partial m_k/\partial t = 4C_k^{ii}$. In order to substitute D_0, D_1, D_2, E_1, and E_2 into eqs. (1) and (2), and set $u_1 = u_2 = m_1/m_0$, $r = 1$. The right side of new equation just equals 4 times of eq. (7), which is consistent with the analysis.

For numerical tests, two simple bimodal cases are performed, taking account both the single point and multipoint expansion. Both initial PSD satisfy the log-normal distribution:

$$N(v,t) = N_0 \exp[-\ln^2(v/v_g)/(2w_g^2)]/(\sqrt{2\pi} v w_g) \tag{10}$$

For case I $N_0^i = N_0^j = 1.0$, $v_g^i = v_g^j = \sqrt{3}/2$, $w_g^i = w_g^j = [\ln(4/3)]^{1/2}$ [14], which represents a mono-modal system and the PSD is separated into two equal sub-PSD. For case II, $N_0^i = 1.0$, $v_g^i = \sqrt{3}/2$, $w_g^i = [\ln(4/3)]^{1/2}$ and $N_0^j = 0.1N_0^i$, $v_g^j = 100v_g^i$, and $w_g^j = 0.1w_g^j$, which represents two log-normal sub-PSD.

Figure 1 shows the results of case I for both single point TEMOM and multi point TEMOM. From the figure, a good agreement is obtain. This is because the particle system is, in the final analysis, a mono-modal system. The consistence between two methods is just as the same as the analysis at the beginning of this paragraph.

Figure 2 shows the results of case II for both single point TEMOM and multi point TEMOM. From the figure, an obvious deviation is found.

It shows that, for a typical bimodal system, the particle size difference between different models cannot be neglected.

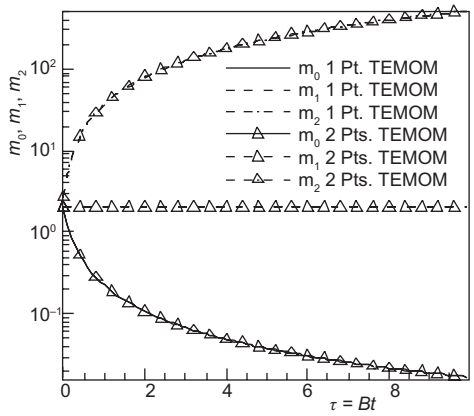

Figure 1. The evolution of moments for case I using different schemes

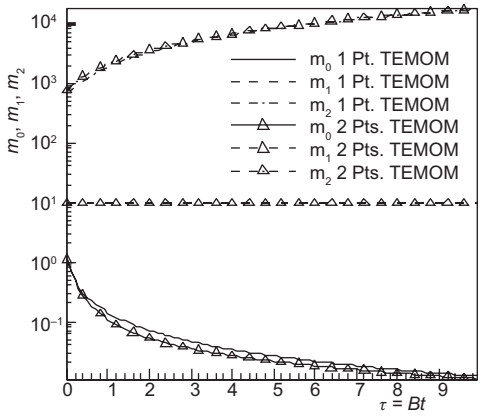

Figure 2. The evolution of moments for case II using different schemes

Conclusions

The current research showed a multipoint Taylor-expansion method of moments for the bimodal particle system. A theoretical deduction was performed and the brief result is given out. A theoretical validation and two following numerical tests are implemented. The result shows that for the mono-modal system, there is almost no difference between the two methods. However, for the bimodal system, the evolution of moments has the same tendency and there is obvious deviation between two methods. The accuracy and stability of current model should also be further discussed.

Acknowledgments

The authors gratefully acknowledge the financial support from the National Natural Science Foundation of China with Grant No. 11302070, the National Basic Research Program of China (973 Program) with Grant No. 2010CB227102.

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Paper submitted: March 15, 2013
Paper revised: May 1, 2013
Paper accepted: May 2, 2013