A numerical method for integrating the kinetic equations of droplet spectra

evolution by condensation/evaporation and by coalescence/breakup processes

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Abstract

An extension of the method of moments is developed for the numerical integration of the kinetic equations of droplet spectra evolution by condensation/evaporation and by coalescence/breakup processes. The number density function $n_k(x,t)$ in each separate droplet packet between droplet mass grid points (x_k, x_{k+1}) is represented by an expansion in orthogonal polynomials with a given weighting function. In this way droplet number concentrations, liquid water contents and other moments in each droplet packet are conserved and the problem of solving the kinetic equations is replaced by one of solving a set of coupled differential equations for the number density function moments. The method is tested against existing analytic solutions of the corresponding kinetic equations. Numerical results are obtained for different coalescence/breakup and condensation/evaporation kernels and for different initial droplet spectra. Also droplet mass grid intervals, weighting functions and time steps are varied.

Introduction

There are three major difficulties in numerical computation of droplet spectra evolution by condensation/evaporation and coalescence/breakup processes, which occur as a result of interaction between droplets and vapour-air environment.

a)The relaxation time of condensation/evaporation process is much smaller than the relaxation time of coalescence/breakup process and therefore the numerical computations of these processes require a different time steps.

b)A correct approximation of droplet number density function $n_k(x,t)$ is required in each separate droplet packet between droplet mass grid points (x_k, x_{k+1}). In Berry, s approximation[1,2] of number density function neither the number concentration nor the liquid water content of droplets are conserved. In Bleck's method[3,4] it is impossible to estimate the error of the approximate numerical solution and an assumption is made +, .t in each separate droplet packet all droplets are spread over the whole mass interval (x_k, x_{k+1}). This Bleck's uniform distribution hypothesis gives as a result a significant increase of the mass conversion velocity from small droplets to large drops.

c)The problem of correct computation of water vapour supersaturation taking into account the release of latent heat of condensation/evaporation during the time step used for the numerical computation of the condensation/evaporation processes.

Method of moments

In this study an extension of Bleck's method[3] and of the method of moments [5,6] is developed for numerical integrating the kinetic equations of droplet spectra evolution by condensation/evaporation and coalescence/breakup processes. Each separate droplet mass interval (x_k, x_{k+1}), where $x_{k+1} = sx_k$ is considered as a droplet packet with its own number concentration, liquid water content and other moments. The unknown number density function $n_k(x,t)$ in each droplet packet is represented by an expansion in orthogonal polynomials with a given weighting function

$$n_k(z,t) = W_k(z,t) \sum_{i=0}^{\infty} a_{ik}(t) G_{ik}(z) \qquad (1)$$

where $z = x/x_k$ represents the nondimensional mass of droplets in the packet (x_k, x_{k+1}).
$W_k(z,t)$--weighting function.

$G_{ik}(z)$-are polynomials orthogonal in the range $(1,s)$ with weighting function $W_k(z,t)$.

$a_{ik}(t)$-are the expansion coefficients which are expressed as linear combinations of the number density function moments and depend on the moments of $W_k(z,t)$ as well.

In this way droplets number concentration, liquid water content and other moments are conserved in each separate droplet packet and the problem of solving the kinetic equations is replaced by one of solving an infinitive set of coupled differential equations for the number density function moments.However, approximating $n_k(z,t)$ by means of first L terms of the expansion (1) and also replacing the expansion coefficients $a_{ik}(t)$ by means of linear combinations of number density function moments we obtain a finite set of

coupled differential equations to compute the first L moments of the $n_k(z,t)$[7]. Note that the approximation of the $n_k(z,t)$ by means of the first L terms of the expansion (1) assumes that the expansion coefficients for i $\angle$, $i=L+1$, ... are zero, that is

$$a_{Lk}(t)=0; \quad a_{L+1,k}(t)=0; \quad ...... \qquad (2)$$

By (2) the larger order moments of the number density function may be determined by means of the first L moments of the $n_k(z,t)$.

The accuracy of the approximation of $n_k(z,t)$ by means of the first L terms of the expansion (1) in droplet packet(x_k,x_{k-1}) depends on the choice of $W_k(z,t)$ as well as on the choice of droplet mass grid points. The number density function $n(x,t)$ is a distribution function which in experiments is determined only for the range $(x,x+dx)$. If droplet mass increment dx is much smaller than x, the $n(x,t)$ in each range $(x,x+dx)$ represents a piecewise constant function and an arbitrary moment of $n(x,t)$ in the range $(x,x+dx)$ is expressed by means of the zero-order moment $dN(x,t)=n(x,t)dx$; therefore also the number density function $n(x,t)$ is determined by zero-order moment $dN(x,t)$ and does not depend on the choice of the weighting functions in the range $(x,x+dx)$.

For the numerical computations of the kinetic equations it is impossible to choose droplet mass grid points for which $(x_{k+1}-x_k)$ is much smaller than x_k ; therefore for such grid points the zero-order approximation of the expansion (1) ($L=1$) will be incorrect for an arbitrary weighting function $W_k(z,t)$. So, if for numerical solution of the corresponding kinetic equations we have chosen the droplet mass grid points $x_{k+1}=sx_k$, then we have to define for what value of the grid intervals $(x_{k+1}-x_k)$ the first-order approximation of (1) ($L=2$) will be correct that is will be not dependent on the choice of the weighting function $W_k(z,t)$. It is shown that for s equal or smaller than two the first-order approximation of the expansion (1) that is the approximation of $n_k(z,t)$ by means of the first two moments is sufficiently correct.

The relations are obtained to compute the zero-order and the first-order approximations of the polynomial expansion (1) for an arbitrary range $(1,s)$ and for an arbitrary weighting functions.

It should be noted that the first-order approximation of the expansion (1) ($L=2$) describes not only the case where the droplets in the packet (x_k,x_{k+1}) are spread over the whole mass interval (x_k,x_{k+1}) , but also the case where the droplets in the packet (x_k,x_{k+1}) are located only in the part of the whole mass interval (x_k,x_{k+1})[7] .

Numerical method for integrating the condensation/evaporation kinetic equation

In this study a separate treatment of microphysics of condensation/evaporation process (without advection phenomena) is adopted and this process for sufficiently small time steps is considered as a space-homogenous process. Such consideration is based on the assumption that the time integration is broken up into separate treatment of the dynamic tendency and of the microphysical processes which control the vapour supersaturation field.

Differential equations which describe the microphysics of the droplet spectra evolution by condensation/evaporation processes can be written as:

$$\frac{\partial n(x,t)}{\partial t} + \frac{\partial}{\partial x} \left\{ \left(\frac{dx}{dt}\right) n(x,t) \right\} = 0 \qquad (3)$$

$$\frac{dx}{dt} = K \frac{S(t)x^{2/3} - Bx^{1/3} + \phi(c)x^{2/3}}{x^{1/3} + \xi} \qquad (4)$$

$$S(t) = Q(t) - Q_s(t) \qquad (5)$$

$$Q(t) + L(t) = Q(0) + M(0) \qquad (6)$$

$$\rho_1 c_p \frac{dT}{dt} = L_\theta \frac{dM(t)}{dt} \qquad (7)$$

$$\frac{dQ_s(T)}{dT} = \frac{Q_s(T)}{T} \left(\frac{L_\theta}{R_V T} - 1 \right) \qquad (8)$$

where $S(t)$-water vapour supersaturation; $M(t)$- droplets total liquid water content; $Q(t)$-water vapour density; $Q_s(t)$- water vapour saturation density at temperature $T(t)$. The equation (3) represents the condensation/evaporation kinetic equation;(4)-represents the individual droplet diffusional growth equation which includes the terms due to surface tension (B) and solute effects-$\phi(c)$; (6) represents the mass conservation equation; (7)- the first law of thermodynamics; (8)- the Clapeyron -Clausius equation.

Multiplying (3) by $x^m dx$ and integrating from $x_k(t)$ to $x_{k+1}(t)$, and also taking into account that $n(x,t)dx = n_0(y)dy$ we have the set of number density function moments equations

$$\frac{dM_k^m(t)}{dt} = m \int_{x_k(t)}^{x_{k+1}(t)} x^{m-1} (dx/dt)n(x,t)dx = m \int_{x_k(0)}^{x_{k+1}(0)} (x(y,t))^{m-1} (dx(y,t)/dt)n_0(y)dy \qquad (9)$$

where

$$M_k^m(t) = \int_{x_k(t)}^{x_{k+1}(t)} x^m n(x,t)dx = \int_{x_k(0)}^{x_{k+1}(0)} (x(y,t))^m n_0(y)dy$$

represents the m-order moment of the number density function in the droplet packet with nonfixed grid points ($x_k(t)$, $x_{k+1}(t)$), that is in the droplet packet which for $t=0$ is contained within grid points ($x_k(0)$, $x_{k+1}(0)$) and for time t transfers in the droplet packet ($x_k(t)$, $x_{k+1}(t)$) as a result of the droplets diffusional growth.

For $t=0$ we have initial conditions:

$$n(x,0) = n_0(y); \qquad x(y,0)=y; \qquad x_k(0)=x_k; \qquad x_{k+1}(0)=x_{k+1}$$

From equation (9) we have for $m=0$ and $m=1$

$$\frac{dN_k(t)}{dt} = 0; \qquad \frac{dM_k(t)}{dt} = \int_{x_k(0)}^{x_{k+1}(0)} (dx(y,t)/dt)n_0(y)dy \qquad (10)$$

where $N_k(t) = M_k^0(t)$ and $M_k(t) = M_k^1(t)$ represent the number concentration and liquid water content respectively in the droplet packet with nonfixed grid points $(x_k(t), x_{k+1}(t))$. Using (10) we have for the droplets total liquid water content

$$\frac{dM(t)}{dt} = \sum_{k=1}^{J} \int_{x_k(0)}^{x_{k+1}(0)} (dx(y,t)/dt)n_0(y)dy \qquad (11)$$

where J-the total number of droplet packets.

Picard's method of successive approximations is used for the integration of differential equation (4) with the initial condition for t=0 x=y. It is assumed that the droplet individual diffusional growth rate in the (j+1)-th apprOximation is determined by the droplet mass in j-th approximation. Substituting (4) in (11) and approximating $n_0(y)$ by means of the first two moments $N_k(0)$ and $M_k(0)$ we obtain the first relationship between total liquid water content of droplets and between water vapour supersaturation:

$$\frac{dM^{(j)}(t)}{dt} = S^{(j)}(t)\phi^{(j-1)}(t) + \Psi^{(j-1)}(t)$$

where

$$\phi^{(j-1)}(t) = K \sum_{k=1}^{J} \int_{x_k(0)}^{x_{k+1}(0)} ((x^{(j-1)}(y,t))^{2/3} n_0(y)dy) \Big/ ((x^{(j-1)}(y,t))^{1/3} + R,$$

$$\Psi^{(j-1)}(t) = K \sum_{k=1}^{J} \int_{x_k(0)}^{x_{k+1}(0)} (dy)((-B(x^{(j-1)}(y,t))^{1/3} + \phi(c)(x^{(j-1)}(v,t))^{2/3} n_0(y))/((x^{(j-1)}(y,t))^{1/3} + R))$$

are the condensation/evaporation integrals.

The second relationship between $M^{(j)}(t)$ and $S^{(j)}(t)$ can be derived using the equations (5)-(8). Expanding $Q_s(t)$ in Tailor's series, we have for sufficiently small time steps,(that is for time steps for which ($T(t)-T(0))<< T(0)$ is satisfied)

$$S^{(j)}(t) = S(0)-(1+F)(M^{(j)}(t) -M(0)) \qquad (12)$$

where

$$F=(((Q_s(T(0))L_0)/(r_1 c_p T(0)))((L_0/R_v T(0))-1)$$

and L_0 represents the latent heat of water vaporization. Such an approach gives the possibility to obtain the analytic relationships to compute the unknown values of $x(y,t)$, $x_k(x_k(0),t)$, $M_k(t)$, $M(t)$, $S(t)$, $Q(t)$, $T(t)$, $Q_s(t)$ for sufficiently small time steps τ, $(0<t<\tau_1)$ which may be much smaller than the time step used for the numerical computation · the coalescence/breakup processes. The redistribution of the liquid water mass from the droplet packets between nonfixed grid points $(x_k(t),x_{k+1}(t))$ among the droplet packets located between fixed grid points (x_k,x_{k+1}) which are used for the numerical computation of the coalescence/breakup processes can be computed without too much difficulty.

Note that according to (10) the number concentration $n_k(t)$ in the droplet packets with nonfixed grid points $(x_k(t),x_{k+1}(t))$ is constant and for initial monodisperse droplet spectrum $M(t)=N(0)x(t)$ where $N(0)$ represents the total number concentration of droplets. Therefore for the initial monodisperse droplet spectrum and for the case B=0 and $\phi(c)=0$ in equation (4) there exists the analytic solution of the set of differential equations (4), (11), (12) which may be used for the test of the numerical method developed in this study.

Numerical method for integrating the coalescence/breakup kinetic equation

The coalescence/breakup kinetic equation for the droplet number density function $n(x,t)$ can be written as:

$$\frac{\partial n(x,t)}{\partial t} = -n(x,t)\int_{x_1}^{\infty}\sigma(x,y)n(y,t)dy + \int_{x_1}^{x/2}\sigma(x-y,y)n(x-y,t)n(y,t)dy - n(x,t)P(x) + \int_{x}^{\infty}n(y,t)Q(y,x)P(y)dy \qquad (13)$$

In this equation $\sigma(x,y)$ represents the coalescence kernel for two droplets of mass x and y;

x_1 is the smallest mass in the spectrum of droplets, $P(x)$- the probability that a droplet of mass x will break up during a unit time and $Q(y,x)$-the droplet number density function, formed due to breakup of a parent drop of mass y.

Multiplying (13) by $x^m dx$ and integrating (13) from x_k to $x_{k+1} = sx_k$ yields

$$\frac{\partial M_k^m(t)}{\partial t} = - \int_{x_k}^{sx_k} x^m n(x,t)dx \int_{x_1}^\bullet \sigma(x,y)n(y,t)dy + \int_{x_k}^{sx_k} x^m dx \int_{x_1}^{x/2} \sigma(x-y,y)n(x-y,t)n(y,t)dy$$

$$- \int_{x_k}^{sx_k} x^m n(x,t)P(x)dx + \int_{x_k}^{sx_k} x^m dx \int_x^\bullet n(y,t)Q(y,x)P(y)dy \qquad (14)$$

where

$$M_k^m(t) = \int_{x_k}^{sx_k} x^m n_k(x,t)dx = x_k^m \int_1^s z^m n_k(z,t)dz \qquad (15)$$

represents the m-th order moment of the number density function of droplets in the packet (x_k, x_{k+1}). According to Bleck [3], the first two double integrals on the right side of (14) can be computed sectionally over small areas. Using this idea also for the computation of the last two integrals in (14), we have

$$\frac{\partial M_k^m(t)}{\partial t} = -\sum_{i=1}^J A_{i,k}^m + \sum_{i=1}^{k-1} A_{i,k-1,k}^m + \sum_{i=1}^{k-1} A_{i,k,k}^m + \sum_{i=k}^J B_{i,k}^m - B_k^m \qquad (16)$$

where $k=1, 2,\ldots,J$; J is the number of droplet packets; $m=0, 1, 2,\ldots$; and m is the order of moments. In the set of differential equations (16) $A_{i,k}^m$, $A_{i,k-1,k}^m$, $A_{i,k,k}^m$ are coalescence double integrals which describe the kinetics of the coalescence process. The last two terms in (16) describe the droplet breakup process.

The computation of the coalescence and breakup double integrals requires the values of the unknown number density function $n(x,t)$ in each separate droplet packet. Therefore approximating again the number density function $n_k(z,t)$ by means of the first L terms of the expansion (1) and replacing the expansion coefficients $a_{lk}(t)$ by means of linear combinations of $M_k^m(t)$, we have from (16) a finite set of coupled differential equations to compute the first L moments of the $n_k(z,t)$ in each separate droplet packet.

There exist conservation relations between the coalescence double integrals, which for m=0 and m=1 describe the droplets number concentration conservation and liquid water content conservation respectively during the coalescence interaction between two droplet packets.

The detailed method for numerical integrating of the coalescence/breakup kinetic equation is contained in .

Numerical computations and concluding remarks

The unknown number density function $n_k(z,t)$ in each separate droplet packet (x_k, x_{k+1}) $(x_{k+1}=sx_k)$ is represented by an expansion in orthogonal polynomials with a given weighting function in the range (x_k, x_{k+1}). In this way the problem of solving the condensation/evaporation and coalescence/breakup kinetic equations is replaced by one of solving a set of coupled differential equations for the moments of the number density function $n_k(z,t)$.

The method of moments developed in this study, is tested against existing analytic solutions of the corresponding kinetic equations. Numerical results are obtained for different coalescence/breakup kernels, for different individual droplet diffusional growth rate and for different initial droplets spectra. Also droplet mass grid points intervals, weighting functions and integration time steps are varied.

The results of the numerical computations of the droplet spectra evolution by condensation/evaporation processes indicate that the convergence of the Picard's method of the successive

approximations for the equation (4) for small time intervals is sufficiently rapid. For monodisperse initial droplet spectra a comparison between numerical results computed by the method of this study and between existing analytic solution of droplet spectra evolution by condensation process is made. It is shown that a simultaneous use of the Picard's method and of the method of moments gives reasonable results which are very close to the existing analytic solution.

For the numerical integration of the coupled differential equations for $N_k(t)$ and $M_k(t)$ which are derived from (16), the forward time differencing is adopted. For practical computations the droplet mass grid points $x_{k+1}=2x_k$ are the most convenient. The results of the numerical computations indicate that if the chosen weighting function is close to the unknown number density function $n_k(z,t)$, the difference between numerical results computed by means of the zero-order approximation and by means of the first-order approximation of the expansion (1) is sufficiently small. The results of numerical computations also show that the difference between numerical results computed by means of the first-order approximation of the expansion (1) with different $M_k(z,t)$ is not large and even if the chosen weighting functions are not close to the unknown number density function $n_k(z,t)$, the use of the first-order approximation of the expansion for different $M_k(z,t)$ gives numerical results which are close to the existing analytic solutions. Therefore one important aspect of the method of moments is its ability to estimate for a given kernels the efficiency of the chosen weighting function, that is the sufficiency of the zero-order approximation of the expansion (1) when there is no analytic solution. A preliminary numerical results are obtained to study the influence of the condensation/evaporation processes on the droplet spectra evolution by the coalescence/breakup processes.

Thus, the convergence of the expansion of the number density function $n_k(z,t)$ in terms of orthogonal polynomials with a given weighting functions in the range $(1,s)$ $(s\leq2)$ is sufficiently rapid and for droplet mass grid points $x_{k+1}=sx_k$ $(s\leq2)$ the approximation of $n_k(z,t)$ by means of the first two terms of the expansion (1) is sufficiently correct.

Acknowledgments

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