A STOCHASTIC MODEL FOR THE COLLECTION GROWTH OF ICE PARTICLES IN MIXED-PHASE CLOUDS

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1. INTRODUCTION

Computational problems that arise when treating ice phase microphysics are much more complicated than those encountered in models with warm rain microphysics. Because of that there are only a few mixed phase non-parameterized cloud models based on solving the kinetic equations for size distribution functions of water drops, ice particles and aggregates. Numerical models with various degrees of complexity have been applied extensively in the past to investigate various ice nucleation mechanisms, ice production rates, and their dependence on cloud microphysical structure.

The collection growth of ice particles is one of the most complex problems in mixed-phase microphysics, since the resulting type of particle may be of a type different from the colliding particles. Usually this process is described by a system of kinetic collection equations of great complexity (Khain and Sednev, 1995; Beheng 1978; Alheit et al., 1990; Reisin et al., 1995).

For example, if only aggregates and pristine ice crystals are considered, then the quasi-stochastic equation for aggregates has the form:

$$\frac{\partial f_a(x)}{\partial t} = \int_0^{x/2} K_a(x_c,x)f_a(x_c)f_a(x')dx'$$
$$-f_a(x)\int_0^\infty K_a(x,x')f_a(x')dx'$$
$$+\int_0^x K_{ia}(x_c,x')f_a(x_c)f_i(x')dx'$$
$$+\int_0^{x/2} K_i(x_c,x')f_i(x_c)f_i(x')dx'$$
$$-f_a(x)\int_0^\infty K_{ia}(x,x')f_i(x')dx' \qquad (1)$$

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The first term in (1) is gain term for aggregates colliding with aggregates, the second term is a loss term for aggregates colliding with aggregates, the third term is a gain term for aggregates colliding with ice crystals, term 4 is a gain term for ice crystals colliding with ice crystals and term 5 is a loss term for ice crystals colliding with aggregates.

For pristine ice crystals the quasi-stochastic equation is:

$$\frac{\partial f_i(x)}{\partial t} = -\int_0^{x/2} K_i(x_c,x)f_i(x_c)f_i(x')dx'$$
$$-f_i(x)\int_0^\infty K_{ia}(x,x')f_a(x')dx' \qquad (2)$$

In (2) the first term is a loss term of ice crystals colliding with ice crystals, and the second term is a loss term of ice crystals colliding with aggregates. In equations (1) and (2) $x_c = x - x'$, $f_a(x)$ and $f_i(x)$ are the mass distributions for aggregates and pristine ice crystals and $K_i(x_c,x')$, $K_a(x_c,x')$ and $K_{ia}(x_c,x')$ are the collections kernels for the collisions of aggregates, pristine ice crystals, and aggregates with crystals.

Within the stochastic framework, the aggregation of ice crystals to form snowflakes was previously studied by Westbrook et al. (2004). In Maruyama and Fujiyoshi (2005) a stochastic model for snow aggregation was developed by adding an aggregation model to the Monte Carlo method of Gillespie (1975).

When other hydrometeor types are included in the analysis, the system of quasi-stochastic equations becomes much more complex. For example, Khain and Sednev (1995) included hydrometeors of seven kinds: water drops, plate-like and columnar crystals, dendrites, snowflakes, graupel and hail. To handle the problem, they formulated some rules in case of single acts of particles collisions (Khain and Sednev, 1995).

In order to avoid the solution of the complex quasi-stochastic equations, a stochastic microphysical framework for calculating the

collection growth in a mixed phase cloud is proposed.

The stochastic algorithm of Gillespie (1976) for chemical reactions in the multicomponent formulation proposed by Laurenzi et al. (2002) was used to simulate the kinetic behavior of the particle population. Within this framework, reacting species are defined as ice particles of specific mass and crystal habit. The stochastic algorithm described in this work was previously used to model the evolution of a two-component droplet spectrum.

The proposed stochastic algorithm allows the study of the effect of ice crystal type on collection growth in mixed-phase clouds and could improve cloud parameterizations in models with bulk microphysics.

2. THE MONTE CARLO ALGORITHM

The stochastic framework, models the crystal aggregation as a random, discrete process. In our report, the stochastic algorithm of Gillespie (1976) for chemical reactions was adopted instead of the algorithm previously elaborated for droplet populations (Gillespie, 1975). This algorithm was reformulated to simulate the kinetic behavior of aggregating systems by Laurenzi et al. (2002). In Laurenzi et al. (2002) species are defined as a type of aggregate with a specific size and composition. In our specific case, species are defined as hydrometeors of different types (droplets, ice crystals or aggregates) with specific mass and aerosol composition.

Within this framework, there is a unique index μ for each pair of hydrometeors i, j that may react (collide). For a system with N species $\left(S_1,\ S_{2,}\ ...\ ,S_N\right)$ $\mu \in \dfrac{N(N+1)}{2}$. The set $\{\mu\}$ defines the total "collision" space, and is equal to the total number of possible interactions (collisions). With this set the reaction probability density function $P(\tau,\mu)$ can be determined. This quantity is defined by

$$P(\tau,\mu)d\tau \equiv \{\text{Probability that at}$$
time the next reaction (collision) in volume V will occur in the infinitesimal interval $(t+\tau,\ \ t+\tau+d\tau)$ and will be a μ reaction}.

In Gillespie (1976) this probability density function has been derived for a system of N species as

$$P(\tau,\mu)d\tau = a_\mu \exp\left(-\sum_{j=1}^{\frac{N(N+1)}{2}} a_j \tau\right) \quad (3)$$

Here $\mu \in \dfrac{N(N+1)}{2}$. The functions a_μ are calculated according to

$a(i,j) = V^{-1} K(i,j) X_i X_j dt$ =Pr{probability that two unlike particles i and j with populations (number of particles) X_i and X_j will collide within the inminent time interval} (4)

$a(i,i) = V^{-1} K(i,i) \dfrac{X_i(X_i-1)}{2} dt$ =Pr{Probability that two particles of the same species i with population (number of particles) X_i collide within the inminent time interval} (5)

The reaction probability density function is the basis of the Monte Carlo algorithm. For calculating the evolution of the system, two random numbers τ and μ must be generated. Equation (3) leads directly to the answers of the aforementioned questions. First, what is the probability distribution for times?. Summing $P(\tau,\mu)d\tau$ over all μ (all possible collisions, (reactions)) results in

$$P_1(\tau)d\tau = \sum_{\mu=1}^{\frac{N(N+1)}{2}} a_\mu \exp\left(-\sum_{\nu=1}^{\frac{N(N+1)}{2}} a_\nu \tau\right)$$
$$= \alpha \exp(-\alpha\tau)d\tau \quad (6)$$

with $$\alpha = \sum_{\nu=1}^{\frac{N(N+1)}{2}} a_\nu$$

The probability function for reactions can be obtained in a similar way, by integrating the pdf $P(\tau,\mu)d\tau$ over all τ from 0 to ∞ results in

$$P_2(\mu) = \frac{a_\mu}{\alpha} \quad (7)$$

Equation (4) gives the probability of a particular reaction μ given an interval (τ, τ+dτ). Equation (6) shows that the probability of a reaction (collision) in time follows an exponential distribution, a characteristic of a process in which events occurs randomly in time.

In order to obtain a random pair (τ, μ), according to the probability density function $P(\tau,\mu)$ we first generate a random number r_1

distributed uniformly in the interval [0,1], then, the inversion method to obtain random numbers is applied. In the inversion method this random number is taken as the probability of a reaction in the time period τ according to $P_1(\tau)$. This probability is obtained by integrating $P_1(\tau)$ from 0 to τ:

$$r_1 = \int_0^\tau P_1(x)dx = \int_0^\tau \alpha\exp(-\alpha x)dx = 1 - \exp(-\alpha\tau) \quad (8)$$

Considering that $1-r_1=r^*_1$ is also a uniformly distributed random number in the interval [0,1], then the time τ can be calculated from (8) in the form:

$$\tau = \frac{1}{\alpha}\ln\left(\frac{1}{r_1^*}\right) \quad (9)$$

The reaction number μ is calculated similarly. A random number r_2 uniformly distributed in the interval [0,1] is generated. Then the pdf $P_2(\nu)$ (7) must be integrated over ν until the addition of the μ probability exceeds the random number r_2. The inequality to obtain the reaction index μ has the form (Gillespie, 1976)

$$\sum_{\nu=1}^{\mu-1} a_\nu < r_2\alpha \le \sum_{\nu=1}^{\mu} a_\nu \quad (10)$$

The former results lead to the Gillespie's direct algorithm:
1) Initialize (set initial numbers of species, set t=0, set stopping criteria).
2) Calculate the function a_μ for all μ.
3) Choose τ according to the exponential distribution $P_1(\tau) = \alpha\exp(-\alpha\tau)d\tau$
4) Calculate μ according to the distribution $P_2(\mu) = \dfrac{a_\mu}{\alpha}$.
5) Change the numbers of species to reflect the execution of a reaction.
6) If stopping criteria are not met, go to step 2.

3. SIMULATION RESULTS

In order to check the performance of Monte Carlo algorithm, a simulation was run considering that the only hydrometeor type is droplets. The results from the Monte Carlo algorithm are the averages over 1000 realizations of the stochastic process. For monodisperse initial conditions, we consider a cloud of 1 cm^3 volume, initially containing N_0 droplets of 10 µm. These droplets

were placed in bin 1 of the size distribution. Fig.1 shows a comparison between the Monte Carlo algorithm and analytical solutions of the SCE for a constant collection kernel. The monodisperse initial distribution was set equal to N_0=100 cm^{-3}. As can be observed, the simulations, yielded the same results as the analytical solutions of the SCE.
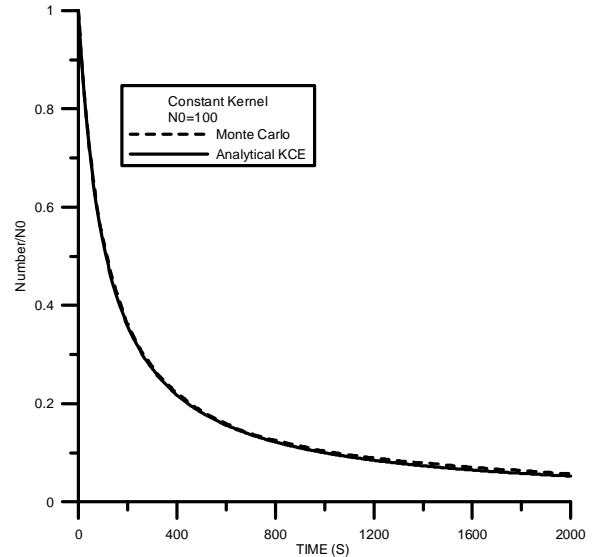

Fig.1. The number of particles averaged over 1000 simulation runs and normalized to the initial number of particles (N_0=100), versus time is shown by the dashed line. The results from the analytical solution are shown by the solid line.

To test the framework for the ice-phase, a simplified simulation was running with hexagonal ice plates and columnar ice crystals for the initial particles. Initial monodisperse distributions with concentrations of 50 cm^{-3} particles for both the columnar ice crystals and hexagonal plates were considered, with masses for the monomer crystals of 10^{-9} and 10^{-10}g respectively. The cloud volume was set equal to 1cm^3. Following Khain and Sednev (1996), the rules in case of single acts of particles collisions for this case are:

- Ice crystal–ice crystal: snowflakes are formed.
- Ice crystal-snowflake: snowflakes are formed.
- Snowflake–snowflake: snowflakes are formed,

Terminal velocity of the hydrometeors were taken from Pruppacher and Klett (1997). The collection efficiency and collection kernels of crystal-ice crystal interactions were parameterized following Khain and Sednev (1995).

Simulations results are the averages over 1000 realizations of the stochastic process (Fig. 2). For the simplified simulation presented in this report, an increase in the snowflake concentration at the beginning of the simulations is observed as a result of the interaction between ice crystals. The posterior reduction is a result of the snowflake–snowflake interaction.
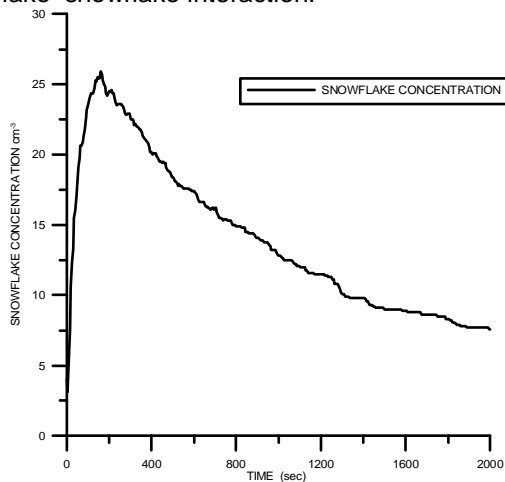

Fig.2. Snowflake concentration averaged over 1000 simulation runs versus time.

To test further the algorithm, a more detailed comparison with averages obtained from solutions of the deterministic quasi-stochastic equations is needed. The collection algorithm described in this work has to be linked with a general microphysical framework, in order to consider all the processs relevant to precipitation formation in mixed phase clouds.

4.   CONCLUSIONS

The stochastic algorithm for chemical reactions developed by Gillespie (1976) in the formulation proposed by Laurenzi et al. (2002) was implemented in order to calculate the time evolution of hydrometeors in a mixed phase cloud. Within this framework, reacting species are defined as hydrometeors of specific mass and type. The collection algorithm described in this work has to be linked with a general microphysical framework, in order to consider all the processs relevant to precipitation formation in mixed phase clouds.

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