Geophysical Laboratory II, academic year: 2023/2024

Modeling collision-coalescence with the Super-Droplet Method

Agnieszka Makulska,
registration number: 417936

tutors: dr Piotr Dziekan and prof. dr hab. Hanna Pawłowska

date of submission: 13 November 2023
date of revision: 22 November 2023

1 Introduction

The exercise concerns modeling the collisional growth of cloud droplets with a Super-Droplet Method in a box model, using algorithms included in the libcloudph++ library. The goal of the exercise is to assess how the mass density function changes with time due to collision-coalescence. The mass density function calculated with the libcloudph++ library is compared with a reference numerical solution of the Smoluchowski equation.

2 Box model

A box model considers an air parcel of a given volume with fixed values of pressure, temperature and relative humidity. Collision-coalescence is the only process considered.

The box simulation is performed using the libcloudph++ library (Arabas et al., 2015). It is a library of algorithms for representing cloud microphysics in numerical cloud models. A Lagrangian particle-based scheme is used, which allows to track the properties of particles during the simulation. It is an implementation of the Super-Droplet Method (Shima et al., 2009), in which particles are represented by super-droplets. Each super-droplet represents a number of droplets with the same dry radius r_d, wet radius r, hygroscopicity κ and position. The multiplicity (the number of droplets represented by a super-droplet), can be different for each super-droplet, and it is time dependent due to coalescence. Super-droplets are assumed to be distributed uniformly in space. The super-droplet is a kind of coarse-grained view of droplets both in the real-space and in the attribute space (Shima et al., 2009).

Sizes and multiplicities of super-droplets are assigned based on a probability density function. The probability density of droplet concentration $n(v)$, depending on the volume v of particle having radius r, is given by an exponential distribution:

$$n(v) = \frac{n_0}{v_0}\, exp\left(\frac{-v}{v_0}\right), \tag{1}$$

where n_0 is the total droplet concentration and $v_0 = 4\pi/3\ r_0^3$ is the volume corresponding to the maximum of the distribution. Equation 1 is equivalent to the probability density of droplet concentration depending on the radius (considering that $n(v)dv = n(r)dr$):

$$n(r) = 3n_0 \frac{r^2}{r_0^3} exp\left(\frac{-r^3}{r_0^3}\right), \tag{2}$$

which can be expressed as a function of the logarithm of the radius, considering that $n(r)dr = n(lnr)d(lnr)$, and thus:

$$n(lnr) = 3n_0 \frac{r^3}{r_0^3} exp\left(\frac{-r^3}{r_0^3}\right). \tag{3}$$

The value of the hygroscopicity is set to $\kappa = 10^{-10} \approx 0$, and thus no solute inside the droplets is considered. This is because the exercise does not concern the activation or condensational growth of droplets. The initial droplet size distribution is presented in figure 1.

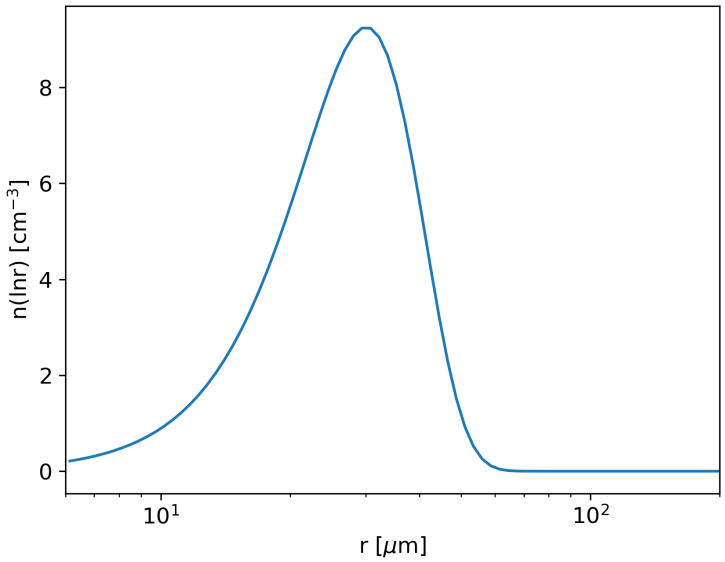

Figure 1: The initial droplet size distribution, described by an exponential function with $n_0 = 2^{23}$ m^{-3} and $r_0 = 30.084$ μm. It is similar to the droplet size distribution in Shima et al. (2009).

The number of super-droplets N_{SD} is prescribed and each super-droplet has a different multiplicity, as described in Dziekan and Pawlowska (2017). The droplet size distribution is divided into N_{SD} bins, with equal sizes on a logarithmic scale. The radius of a single super-droplet is randomly selected within each bin. The first step of the initialization is to find the largest and the smallest initial radii, r_{max} and r_{min}. They are found iteratively, starting with initial values. The requirement is that the particle multiplicity in bins corresponding to both r_{min} and r_{max} must be greater than or equal to 1. In each iteration, if r_{min} (or r_{max}) does not satisfy the requirement, it is increased (decreased) by 1 %. This method does not represent the tails of the distribution well, because increasing the number of bins, N_{SD}, causes the width of each bin to decrease and this in turn gives relatively large values of r_{min} and relatively small values of r_{max} (in order to satisfy the requirement of particle multiplicity greater than 1). Since the large tail of the distribution is important for coalescence, an additional "large tail" option is added in the libcloudph++ library. If this option is used, additional super-droplets with multiplicity 1 and radii $r > r_{max}$ are created. This makes the actual number of super-droplets higher than the prescribed N_{SD}, typically by ca. 1 %. There is no such procedure for the small tail of the distribution, because very small droplets are not important for coalescence.

A simulation of a box with the volume 100 m^3 is run for the time of 1800 s, with the time step of 1 s. The number of super-droplets is initially set to 10^5, but additional 516 super-droplets are added by considering the droplet size distribution with a "large tail" option. The terminal velocity of droplets is modeled with semi-empirical formulas from Beard (1976). The formulas consider hydrodynamic effects of the flow on the motion of droplets. The collision-coalescence is modeled with a gravitational kernel, with efficiencies from Davis (1972) for small droplets and from Hall (1980) for large droplets. They include hydrodynamic interactions between droplets, which take into account the effect that a smaller droplet can be swept aside by the stream flow around the larger droplet or bounce on the surface, which reduces the probability of collision.

3 Super-Droplet Method

In the Super-Droplet Method, the coalescence probability P_{jk}^S for two super-droplets with multiplicities ξ_j and ξ_k and radii r_j and r_k is defined in the following way:

$$P_{jk}^S = max(\xi_j, \xi_k) P_{jk}, \tag{4}$$

where P_{jk} is the probability of coalescence of two real droplets with radii r_j and r_k , given by

$$P_{jk} = K(r_j, r_k) \frac{\Delta t}{\Delta V}, \tag{5}$$

where $K(r_j, r_k)$ is the coalescence kernel for the two droplets, ΔV is the volume of the region with the droplets and Δt is the time interval.

In the simulation, the collision-coalescence of super-droplets is solved with the Monte Carlo scheme. From n_s super-droplets, a list of randomly chosen, non-overlapping pairs is generated. Non-overlapping means that no super-droplet belongs to more than one pair. By examining only these $[n_s/2]$ pairs ($[n_s/2]$ is the floor function of $n_s/2$), instead of all possible $n_s(n_s\text{-}1)/2$ pairs, the computational cost is decreased. In compensation for this simplification, the coalescence probability is multiplied by the ratio of pair numbers, and the corrected, scaled up probability of coalescence p_α for the α-th pair is obtained as:

$$p_\alpha = P_{j_\alpha k_\alpha}^S \frac{n_s(n_s-1)}{2} \Bigg/ \left[\frac{n_s}{2}\right], \tag{6}$$

where $P_{j_\alpha k_\alpha}^S$ is the coalescence probability given by equation 4.

For each pair of super-droplets, a random number from a uniform distribution between 0 and 1 is generated. If the random number is smaller than the probability of coalescence, the two super-droplets coalesce. Otherwise, they do not coalesce. Let us consider the coalescence of two super-droplets with multiplicities ξ_j and ξ_k and radii r_j and r_k, respectively. This process is realised in the following way: if $\xi_j \neq \xi_k$, then $\xi_j > \xi_k$ can be chosen without losing generality, and only the $min(\xi_j, \xi_k)$ pairs of droplets contribute to the coalescence of the super-droplet pair. After a collision event, multiplicities and radii of super-droplets become:

$$\xi_j' = \xi_j - \xi_k, \quad \xi_k' = \xi_k, \tag{7}$$

$$r_j' = r_j, \quad r_k' = (r_j^3 + r_k^3)^{1/3}, \tag{8}$$

where ξ_j' and ξ_k' are multiplicities of super-droplets after the collision and r_j' and r_k' are radii of super-droplets after the collision. If $\xi_j = \xi_k$, then all of the droplets contribute to the coalescence of the super-droplet pair. Unlike in the formulation of Shima et al. (2009), in this case one of the particles is left with zero multiplicity. Particles with zero multiplicity are "recycled" - properties of particles with the highest multiplicities are assigned to recycled particles, halving the multiplicity. Attributes other than the wet radius are summed (extensive attributes such as the dry volume) or averaged (intensive attributes such as the hygroscopicity).

4 Solution of the Smoluchowski equation

The stochastic coalescence equation (also called the Smoluchowski equation) describes the rate of change of number distribution of droplets having volume X due to collisions:

$$\frac{\partial n(X,t)}{\partial t} = \frac{1}{2}\int_0^X dX' n(X') n(X-X') K(X', X-X') - n(X)\int_0^\infty dX' n(X') K(X, X'), \tag{9}$$

where $n(X)$ is the probability density of droplet concentration, $X = (4\pi/3)r^3$ is the volume of a droplet with radius r and K is the coalescence kernel.

Results of the Smoluchowski equation can be represented by a mass density function $g(lnr)$. It is defined in such a way that $g(lnr)d(lnr)$ is the mass of water per volume, in droplets with radii between r and $r + d(lnr)$. The results depend on the choice of the coalescence kernel. Analytic solution is not available for the kernel used in this exercise. The reference solution for the mass density function is generated numerically using the Exponential Flux Method developed by Bott (1998).

The libcloudph++ library provides an estimator for the mass density function, which is based on the estimator function defined in Shima et al. (2009). Results obtained with the libcloudph++ library are compared with the reference solution of the Smoluchowski equation.

5 Results

Figure 2 shows the evolution of the mass density function assessed in the box simulation described in section 2. The mass density function is assessed with an estimator included in the libcloudph++ library. Results at the end of the simulation are compared to the reference solution of the Smoluchowski equation after the time t = 1800 s. The root mean square deviation, $RMSD$, between the results and the reference solution is calculated. $RMSD$ is defined as

$$RMSD = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i - \hat{x}_i)^2}\ , \tag{10}$$

where N is the number of data points, x_i are the observed values and $\hat{x}_i$ are the reference values.

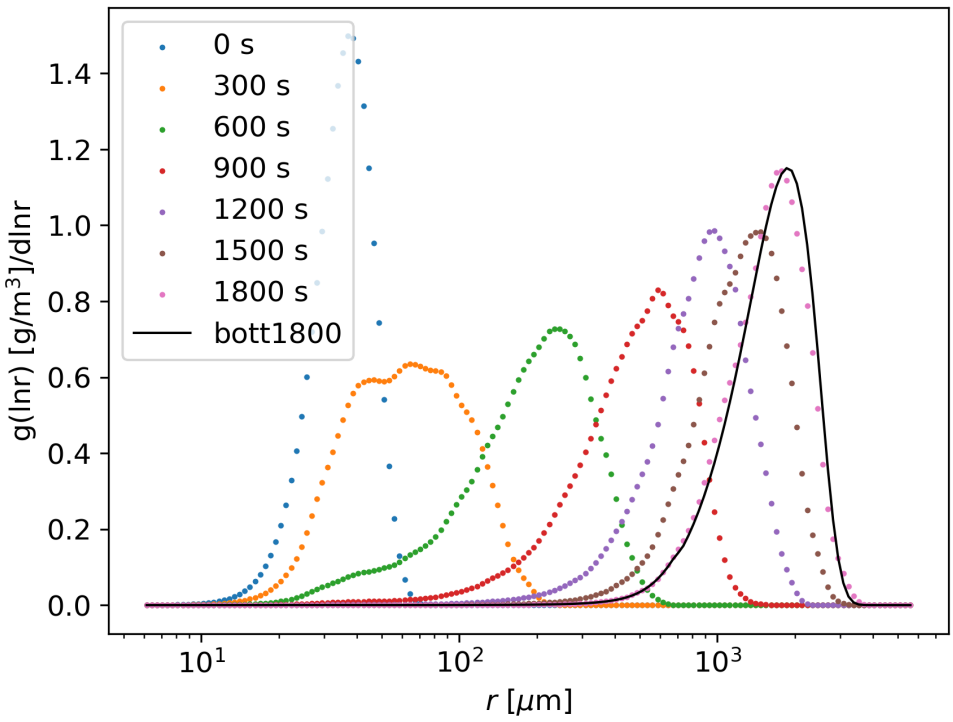

Figure 2: The mass density function assessed in the simulation at different instants of time (marked with color dots). The black line (bott1800) is the solution of the Smoluchowski equation at the time t = 1800 s.

With increasing time of the simulation, the mass density function is shifted towards larger radii. The root mean square deviation between the mass density function assessed in the simulation and the solution of the Smoluchowski equation at t = 1800 s is equal to 0.036 (g/m^3)/dlnr. Thus, the result of the simulation agrees with the solution of the Smoluchowski equation, with a small error.

Figure 3 shows the evolution of the mass density function, calculated from the third moment of the droplet size distribution assessed in the simulation. The third moment of the droplet size distribution, M_3, is defined as

$$M_3 = \int_r^{r+dlnr} r^3 n(r) dr, \tag{11}$$

which is proportional to the total volume of droplets having radii between r and $r + dlnr$. The calculation of the mass density function is done in the following way:

$$g(lnr)\ d(lnr) = \frac{4}{3}\pi M_3(r)\rho_l, \tag{12}$$

where ρ_l is the density of liquid water. By rearranging equation 12 one gets the following equation:

$$g(lnr) = \frac{4}{3}\pi M_3(r)\rho_l \frac{1}{dlnr}\ . \tag{13}$$

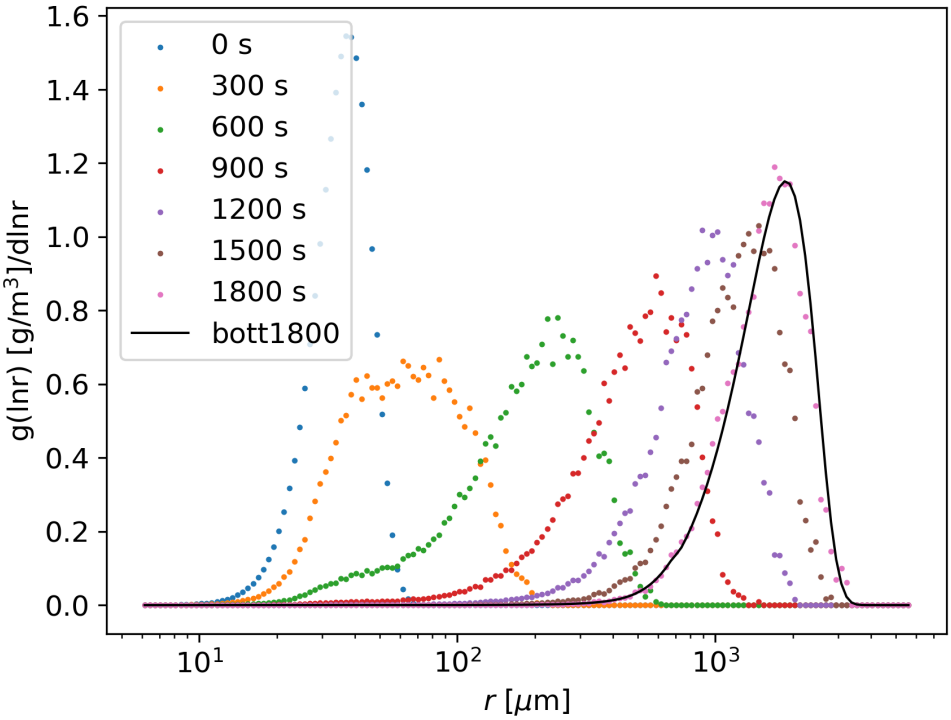

Figure 3: The mass density function calculated from the third moment of the droplet size distribution, at different instants of time (marked with color dots). The black line (bott1800) is the solution of the Smoluchowski equation at the time t = 1800 s.

The mass density function calculated from the third moment of the droplet size distribution is almost the same as the mass density function assessed with the estimator. The root mean square deviation between the mass density function calculated from the third moment and the solution of the Smoluchowski equation at t = 1800 s is equal to 0.040 g/(m^3 dlnr). This is slightly larger than the deviation between the mass density function assessed with the estimator and the reference result.

Figure 4 shows radii of the super-droplets, for different times of the simulation.

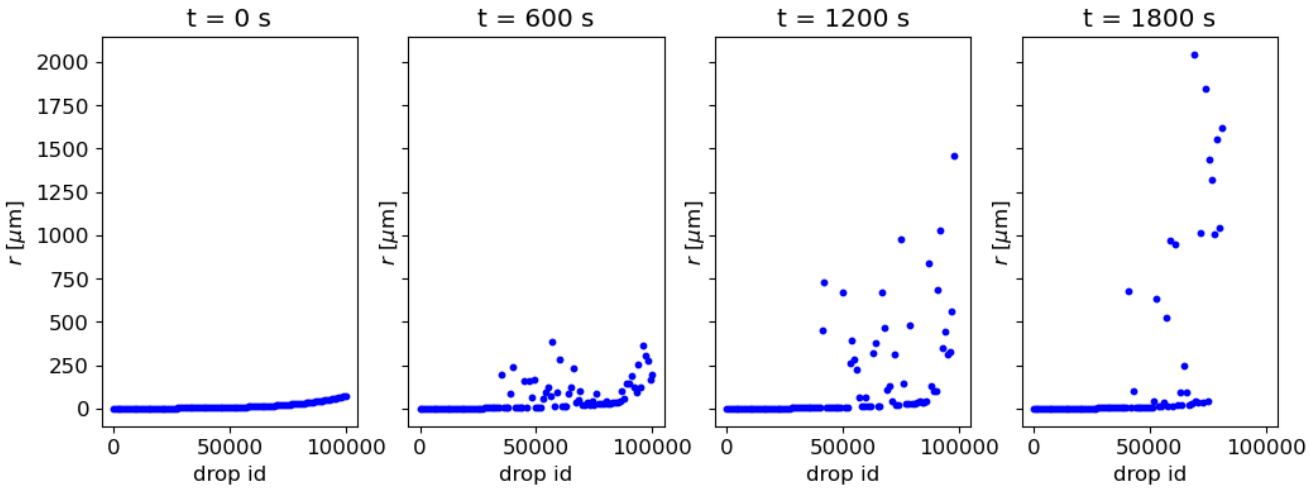

Figure 4: Radii of super-droplets, for selected simulation times. Each point represents a single super-droplet.

As a result of the collision-coalescence, radii of many super-droplets increase in time, as the number of super-droplets decreases, from 100516 at the time t = 0, to 81209 at the time t = 1800 s. At the time t = 0, radii of all super-droplets are smaller than 100 μm. At the time t = 1800 s, some super-droplets reach radii up to 2 mm.

6 Conclusions

The time evolution of the mass density function was assessed in a box model, in which collision-coalescence was the only process modeled. The simulation was run with algorithms included in the libcloudph++ library. Results were compared with a reference solution of the Smoluchowski equation. It was found that the results agree with the reference solution, with a small error. The mass density function was calculated from the third moment of droplet size distribution. The results agreed with the reference solution, with a slightly larger error than the mass density function calculated with the estimator included in the libcloudph++ library. Radii of individual super-droplets were calculated and it was shown how they increse during the simulation.

References

Arabas, S., Jaruga, A., Pawlowska, H., & Grabowski, W. W. (2015). Libcloudph++ 1.0: A single-moment bulk, double-moment bulk, and particle-based warm-rain microphysics library in c++. *Geoscientific Model Development*, *8*(6), 1677–1707. https://doi.org/10.5194/gmd-8-1677-2015 (cit. on p. 2).

Beard, K. V. (1976). Terminal velocity and shape of cloud and precipitation drops aloft. *Journal of Atmospheric Sciences*, *33*(5), 851–864. https://doi.org/https://doi.org/10.1175/1520-0469(1976)033⟨0851:TVASOC⟩2.0.CO;2 (cit. on p. 3).

Bott, A. (1998). A flux method for the numerical solution of the stochastic collection equation. *Journal of the Atmospheric Sciences*, *55*(13), 2284–2293. https://doi.org/https://doi.org/10.1175/1520-0469(1998)055⟨2284:AFMFTN⟩2.0.CO;2 (cit. on p. 5).

Davis, M. H. (1972). Collisions of small cloud droplets: Gas kinetic effects. *Journal of Atmospheric Sciences*, *29*(5), 911–915. https://doi.org/https://doi.org/10.1175/1520-0469(1972)029⟨0911:COSCDG⟩2.0.CO;2 (cit. on p. 3).

Dziekan, P., & Pawlowska, H. (2017). Stochastic coalescence in lagrangian cloud microphysics. *Atmospheric Chemistry and Physics*, *17*(22), 13509–13520. https://doi.org/10.5194/acp-17-13509-2017 (cit. on p. 3).

Hall, W. D. (1980). A detailed microphysical model within a two-dimensional dynamic framework: Model description and preliminary results. *Journal of Atmospheric Sciences*, *37*(11), 2486–2507. https://doi.org/https://doi.org/10.1175/1520-0469(1980)037⟨2486:ADMMWA⟩2.0.CO;2 (cit. on p. 3).

Shima, S., Kusano, K., Kawano, A., Sugiyama, T., & Kawahara, S. (2009). The super-droplet method for the numerical simulation of clouds and precipitation: A particle-based and probabilistic microphysics model coupled with a non-hydrostatic model. *Quarterly Journal of the Royal Meteorological Society*, *135*(642), 1307–1320. https://doi.org/10.1002/qj.441 (cit. on pp. 2–5).