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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Monte Carlo simulations of two-component drop growth by stochastic coalescence" *by* L. Alfonso et al.

L. Alfonso et al.

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First, we would like to thank the anonymous reviewers for their comments that will improve the quality of our paper. Our revised version will include several of their suggestions.

Reply to anonymous referee # 2

1) Section 3.1 (Comparison of the Monte Carlo algorithm with analytical solutions):

Yes, section 3.1 does not have any new results, but there are some differences with the results outlined in Laurenzi et al. (2002), since the solutions were calculated for the constant polynomial kernel obtained by Long (1974). The other issue is the averaging.

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Laurenzi et al. (2002) performed the simulations with a large number of particles for the two initial species (10 000 and 20 000), and run only a single stochastic experiment (infinite system approximation). In our case the initial number of particles was 60, and the average was calculated over 1000 realizations.

2) Section 3.1 (Simulations with realistic initial distributions and hydrodynamic kernel):

The peaks observed in figures 11 and 12 are not consequences of the gelation since the solutions displayed are the averages calculated from the Monte Carlo algorithm, not the solutions obtained from the numerical integration of the kinetic collection equation. This is an important issue, since in certain situations the Monte Carlo averages and the solutions of the mean field kinetic collection equation are different (for example, after the breakdown time or in the presence of correlations). As we know, the stochastic algorithm conserves mass (Laurenzi et al., 2002, Alfonso et al. 2008). The failure to conserve mass after the breakdown time (gelling transition) observed in the kinetic collection equation for the product kernel, is not observed in the stochastic simulations. This is illustrated and analyzed in the figure 12 of Alfonso et al. (2008), where the total mass calculated from the stochastic algorithm is compared with the total mass calculated from the kinetic collection equation for both the sum and product kernels. As can be observed in Figure 12 of Alfonso et al. (2008), the stochastic algorithm conserves mass after the breakdown time.

On the other hand, the kinetic collection equation is always valid when the Long's kernel is used (there is no gelling transition for the Long's kernel) as was analyzed by Long (1974). He approximated the hydrodynamic kernel by two separate polynomials:

$9.44 \times 10^9 (x^2 + y^2)$if $R \leq 50\mu$m

or by

$5.78 \times 10^3 (x + y)$if $R > 50\mu$m

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In the former expression, *x* and *y* are volumes of the colliding droplets, and *R* is the radius of the largest colliding droplet. As we know, the *xy* term predicts too rapid growth for the large drops in the cloud. Then, if the first polynomial is extrapolated to sufficiently larger droplet sizes it will be many times larger than the hydrodynamic kernel, and the kinetic collection equation will be no longer valid. The problem is avoided by changing to the linear version of the polynomial if $R > 50\mu m$. Because *K(x,y)* is linear for *R*>50 μm, then the validity time will be infinite for this case (Long, 1974). By doing this, he avoided the inclusion of non-physical *xy* terms and the breakdown of the KCE will be avoided, since its solutions are valid for kernels of the type *B(x+y)* for all times. **To remark the bimodality of the distributions, the 2-D distribution will be plotted in an additional figure in the revised version.**

3) Page 7292:

Actually *N(m,n;t)* is the average concentration of the particles consisting of m and n monomers of the first and the second kind respectively (*m,n* mers), not the number of species (type of particles with drop mass , and aerosol mass). This will be corrected in the revised version of the manuscript.

For each of the *N(m,n;t)* particles, the water mass equals the mass of the smallest (monomer droplet) multiplied by *m*, and the aerosol mass for each particle equals the mass of the smallest (monomer aerosol) multiplied by *n*. Species are the type of particles with a given m,n combination. For example, *N(2,1;0)*=1000 means that as an initial condition we have 1000 particles (not species), all of them with a water mass that is twice the mass of the monomer droplet (in our simulation the monomer droplet is 10 μm in radius, droplet mass 4.18810^{-9}g) and with aerosol mass that equals the mass of the monomer aerosol (1.1410^{-14}g). Then, the total mass of each particle will be $2 \times 4.188 \times 10^{-9} g + 1.14 \times 10^{-14} g$. In this case, at the beginning of the simulation we have 1000 particles but only one specie (the one for the combination 2,1).

The number of bins required for a given run will depend on the number of species

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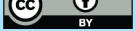

generated during the simulation. We will need 1000 bins in one component only if we have minimum 1000 species (not 1000 particles). In the simulations, the number of species is actually not very large, which is very good from the computational point of view. For example, for a simulation experiment with two species and 300 particles at t=0 (*N(1,1;0)*=100 and *N(1,2;0)*=200) with a constant kernel (*K(m,n;*m_1*,*n_1*)* =1.2x10-4 $cm^3 s^{-1}$), the total number of species created during the 3000 s of the simulation for one realization of the Monte Carlo algorithm was 82. That means that 82 different type of particles were generated during the process.

In the stochastic simulations the mass is always conserved, even for gelling kernels. This fact is discussed in detailed in Laurenzi et al. (2002) and in Alfonso et al. (2008). If the initial condition is *N(2,1;0)=1000* , then after one collision, the number of particles for the species with (2,1)-mers change to reflect the execution of collision. In this case the new number of particles in the species with (2,1)-mers will 998, and a new species with the combination (4,2) will be created. The number of particles in this specie is 1.

The equation (4) of the paper reflects this process: $A_{2,1} + B_{2,1} = C_{2+2,1+1}$. Then, the new droplet is placed in the grid box with index (4,2). At this stage, there is 2 species and 999 particles in the system. The new droplets that are generated are always placed in bins that are exactly a multiple of the mass of the monomer droplet and the monomer aerosol, and the total mass is conserved, with no need to interpolate. In the revised version, the binning will be described in greater detail as suggested by the referee.

4) Yes, in his paper Long (1974) uses the volume of colliding droplets in cubic centimeters. In our paper we use the masses of both droplets and aerosols in grams. Then, in the equations 19 and 20 $x_{species}(i)$ are in grams and the units of the constants in the polynomial approximation are modified to reflect this change. For the first approximating polynomial in the Long's kernel the coefficient (9.44×10^9) has units cm^3 g^{-2} s^{-1}. For the second approximating polynomial the constant (5.78×10^3) has units cm^3 g^{-1} s^{-1} . In all the simulations, the cloud volume was set equal to 1 cm^3. **All these questions will be discussed in more detailed in the revised version as suggested**

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by the referee.

References:

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