Collisional breakup with constant super-droplet number

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Here we describe some results of numerical experiments with different implementations of collisional breakup in a super-droplet code of the collision-coalescence-breakup equation. This contributes to a discussion of the manuscript *'Breakups are Complicated: An Efficient Representation of Collisional Breakup in the Superdroplet Method'* (de Jong et al., 2022). The goal is an implementation of collisional breakup with a constant number of super-droplets (SDs). Due to the nature of collisional breakup to produce many droplets of very different sizes from a single collision event, such an implementation is not straightforward.

Collisional breakup in McSnow

The Monte-Carlo Lagrangian particle model McSnow of Brdar and Seifert (2018) is based on the super-droplet algorithm of Shima et al. (2009). In McSnow collisional breakup of raindrops is implemented as described in the Appendix of Bringi et al. (2020). The implementation makes use of the empirical parameterizations of Low and List (1982) in the formulation of McFarquhar (2004). Using the equations of McFarquhar (2004) greatly simplifies the implementation compared to the original Low and List scheme. The implementation as described in Bringi et al. (2020) does create new super-droplets during collisional breakup. This seems necessary, especially because it is in fact only one super-droplet available to describe the outcome of the breakup event. Given the fact that breakup can lead to two or three distinct fragment modes, it seems rather difficult to achieve an accurate description with a constant number of SDs. In McSnow a merging algorithm limits the number of SDs afterwards. This requires some additional tuning of the criteria of the merging algorithm. The merging also adds some computational cost which scales with $\mathcal{N}\log(\mathcal{N})$, where $\mathcal{N}$ is the number of SDs in a grid box. Hence, a breakup algorithm with a constant number of SDs would be desirable.

For a given collision of two droplets with drop diameters D_1 and D_2, masses m_1 and m_2 and multiplicities ξ_1 and ξ_2, the super-droplet implementation of collisional breakup provides the masses (and diameters) and the number of the collision fragments in each mode of the fragment distribution function (FDF). For filament breakup these are three fragment modes for the other breakup types (disc and sheet breakup) two different fragment modes occur. The diameters d_i of the collision fragments are sampled from the empirical FDF. The mass of the drop during (temporary) coalescence is $m_{\text{coal}} = m_1 + m_2$ with a corresponding diameter d_{coal}.

Implementation of constant-SD breakup in McSnow

Here and in the following we assume $\xi_1 > \xi_2$. Then the SD with diameter D_1 is used for the $\xi_1 - \xi_2$ drops that do not participate in the collision event. Hence

$$m_1' = m_1 \tag{1}$$

$$\xi_1' \ = \xi_1 - \xi_2 \tag{2}$$

where the prime denotes quantities after the collision event and m is the drop mass.

The main idea of the constant-SD breakup is a stochastic sampling of the fragment mode. Here we test two implementations. First, a number-weighted probability sampling as suggested by de Jong et al. (2022). An alternative is a sampling that is proportional to the mass of the fragments. Hence, bigger drops are chosen more often. A third viable implementation would be an equal probability sampling of the fragment modes, but this ends up being quite similar to the number-weighted algorithm and is therefore not included in the following discussion.
The number of fragments in each fragment mode is n_i and the diameter, which has already been sampled from the FDF for that fragment mode, is d_i. Note that n_i can be zero if a fragment mode does not exist (sheet and disc breakup). The mass-weighted sampling is implemented as given in Algorithm 1. This stochastic sampling provides the index i of the fragment mode that is then represented by the super-droplet.
For both, number-weighted and mass-weighted sampling, the mass and multiplicity of the second super-droplet is then specified as

$$m_2' = \frac{\pi}{6}\rho_l\, d_i^3 \tag{3}$$

$$\xi_2' = \frac{m_{\mathrm{coal}}}{m_2'} = \frac{m_1 + m_2}{m_2'} \tag{4}$$

where ρ_l is the density of liquid water. The multiplicity ξ_2' has to be specified by the coalesced mass to ensure mass conservation. Hence, the only information that survives from the breakup parameterization is the diameter d_i that has been sampled from the corresponding mode of the FDF and - more subtle - the probability of occurence of that mode and that specific drop size.

Algorithm 1: Stochastic fragment mode selection in mass-weighted constant-SD breakup

```
p_1 = n_1 (d_1/d_coal)^3
p_2 = n_2 (d_2/d_coal)^3 + p_1
call random(r)                    ; uniform random variable in [0,1]
if r < p_1 then
    i = 1
else if r < p_2 then
    i = 2
else
    i = 3
```

On one hand, the mass-weighted sampling may look somewhat arbitrary at first, but on the other hand the number-weighted sampling can sometimes produce an unreasonable large number of small drops because the coalesced mass m_{coal} has to be represented by very many tiny droplets of the same size. The fact that ξ_2' is specified by the coalesced mass is another argument to favor the mass-weighted sampling. But *a priori* it is not obvious whether number-weighted or mass-weighted sampling will give the correct solution, if any of the two.
In the following, we compare with the merging-based breakup algorithm of McSnow that does no stochastic mode selection and simply creates super-droplets for all fragments. Those can then be merged in a second step to limit the number of super-droplets. Hence, the merging-based breakup algorithm can serve as a benchmark simulation, especially if the number of super-droplets is large.

Collisional breakup simulations with McSnow

We present zero-dimensional box model simulations of the coalescence-breakup equation (similar to section 3.1 of de Jong et al. (2022). The initial condition is a Gamma distribution in drop

mass with a shape parameter of 1, a liquid water content of 2.5 g/m^3 and an inital mean mass of $\bar{m}_0 = 3 \times 10^{-10}$ kg. Simulations are performed for 7200 s with a time step of 1 s. The binning of the drop size distribution is done with the kernel density estimator described in Section 5.1.4 of Shima et al. (2009) using $\sigma_0 = 0.62$.
Figure 1 shows the quasi-equilibrium drop distributions reached after 7200 s as number and mass density distributions for different number of super-droplets (SDs) ranging from $\mathcal{N} = 10^6$ over $\mathcal{N} = 4192$ to $\mathcal{N} = 120$. The notation $f(D)$ and $g(\ln r)$ follows Berry and Reinhardt (1974) and $g(\ln r)$ should be equivalent to the $\mathrm{d}m/\mathrm{dln}\, r$ distribution of de Jong et al. (their Figs. 3-5).
The results for $f(D)$ of the merging-based algorithm and the mass-weighted constant-SD algorithm compare reasonably well with each other and with Figure 15 of McFarquhar (2004). In the simulations with high SD number, the mass-weighted constant-SD algorithm exhibits a more pronounced peak from small (filament) droplets compared to the merging-based simulations. Since there is no convergence of the two algorithms to the same solution, it is not clear which simulation is better. The large drop tail of the distributions agrees remarkably well for those two algorithms. For $\mathcal{N} = 120$ both algorithms show a smaller slope of the drop distribution with much larger drops. The number-weighted sampling, on the other hand, gives a much too narrow distribution and does not even converge to a similar distribution as the other two algorithms. This suggests that the number-weighted sampling is generally biased towards small droplets and does not give the correct solution. Hence, the mass-weighted stochastic mode selection seems to be the method of choice for a constant-SD implementation of collisional breakup in a super-droplet algorithm.

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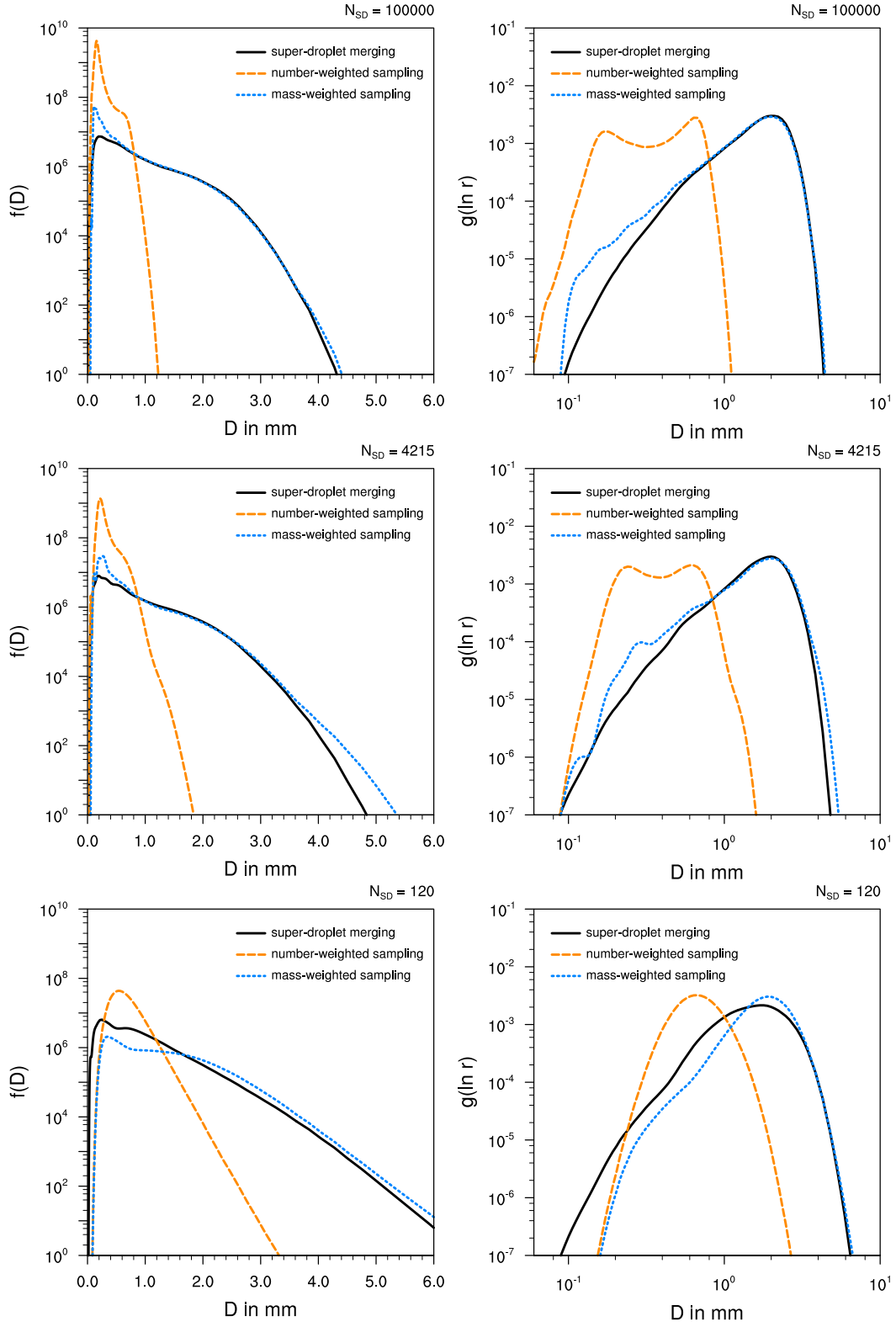

Figure 1: Quasi-equilibrium drops size distributions. Number distributions (left), mass distributions (right), the number of SDs decreases from top to bottom.