Effects of Pressure on Collision, Coalescence, and Breakup of Raindrops. Part II: Parameterization and Spectra Evolution at 50 and 100 kPa

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ABSTRACT
Fragment size distributions, experimentally obtained for six drop pairs colliding at 50 kPa, are parameterized similarly to the 100-kPa drop pair experiments by Low and List. This information is then introduced into a box model to allow assessment of the spectra evolution and a comparison of the two datasets taken at the two pressures. The differences in breakup patterns include the following: The contributions to mass transfer by breakup and coalescence are very similar at the two pressures, with larger values at lower pressure; the overall mass evolution is not particularly sensitive to pressure; and disk breakup plays an “erratic” role. The situation for the number concentration, however, is totally different and develops gradually. At 50 kPa there is also no three-peak equilibrium developing as for 100 kPa. The times to reach equilibrium are ~12 h. Note that the box model does not include accretion of cloud droplets—which may well be more important than growth by accretion of fragments.

Application of the new parameterization is not beneficial for low rain rates, but it is strongly recommended for large rain rates (>50 mm h\(^{-1}\)).

1. Introduction
Apparatus, experiments, and results of the breakup of six different drop pairs are presented in List et al. (2009, hereafter Part I), which describes the experimentally determined main breakup patterns as filaments, sheets, and disks. Although three bag breakups had been observed in Low and List (1982, hereafter LL82), none were seen at 50 kPa. Shifts in patterns included the lack of sheet and disk breakup for two drop pairs.

Part II deals with the parameterization of the results at 50 kPa. These approximations are based on physical quantities such as the collision kinetic energy (CKE) and various surface energies, which may play a role in the breakup. This has been the standard approach by McTaggart-Cowan and List (1975), LL82, and Fung (1984), who further refined the parameterization. However, computational stability required further adjustments, such as those carried out by Nissen (1996). This present paper directly follows and details his newest improvements.

Once the individual fragment spectra are described by formulas, a box model can address the spectra evolution. This is being done for both 50 and 100 kPa, both for number and mass concentration. The evolution is then explored and diagrams are presented that address the times required for development into equilibrium distributions, as had been postulated by List (1988). Other studies of spectra evolution are by Gillespie and List (1978), Valdez and Young (1985), List et al. (1987), and List and McFarquhar (1990). Attention is also given to the interplay between accretion and the different types of breakup: filament, sheet, and disk breakup.

2. Parameterization of the 50-kPa fragment size distributions
Other physical quantities are introduced now because they are involved in forthcoming ordering and
parameterizations of events: the collision kinetic energy; the surface energy of the large and small drops, \( S_L \) and \( S_S \); the total surface energy \( S_T \); and \( D_L \) and \( D_S \), the large and small drop spherical equivalent diameters. The surface tension of water, \( \sigma_w \), the sum of both drops, \( \sigma_T = \sigma_w(D_L^2 + D_S^2) \), and \( S_C = \sigma_w(D_L^2 + D_S)^{2/3} \) for the coalesced drop are produced. For 50 kPa and 20°C, the terminal velocities \( V_L \) and \( V_S \) (of the large and small drops, respectively) are based on the equation by Best (1950). The collision kinetic energy for centered mass coordinates is defined as

\[
CKE = \left( \rho_w \sigma_w/12 \right) \frac{D_L^2 D_S^3}{D_L^3 + D_S^3} (V_L - V_S)^2, \tag{1}
\]

where \( \rho_w \) is the density of water. All dimensions are in cgs units as in all previous parameterization papers. Table 1 lists all the properties of the six drop pairs for 50 kPa.

Equation (1) describes a two-body problem, leaving out the third body: the air. This creates an incomplete description of the interactions and it should not be expected that CKE is the controlling factor.

The LL82 parameterization was refined by Fung (1984) and then redone by Nissen (1996) to obtain computational stability. Following Nissen, it is applied to the 50-kPa dataset to describe the histograms of all the breakup types. Using the subscripts \( f \) for film, \( s \) for sheet, and \( d \) for disk, the average number of drop fragments resulting from breakup \( F_b \) is given by

\[
F_b = R_f F_f + R_s F_s + R_d F_d. \tag{2}
\]

where \( R_i \) is the fraction of collisions for a given breakup type. For each collision type at 50 kPa, the fraction \( F_i \) is related to the parameterization for 100 kPa and is given by

\[
F_{f,50} = F_{f,100}(25.7 \text{ CKE}_{100}^{1.9} + 0.205) \quad \text{for} \quad D_S = D_{S0}, \tag{3}
\]

where

\[
D_{S0} = [(F_{f,100} - 2)/(1.02 \times 10^4)]^{1/2.83} \quad \text{(as in LL82)}, \tag{5}
\]

\[
F_{s,50} = F_{s,100}(6.71 S_C^{-0.585} - 0.289), \quad \text{and} \tag{6}
\]

\[
F_{d,50} = F_{d,100}(4.0 S_C^{-0.4} - 0.591). \tag{7}
\]

For the filament and sheet types the 100-kPa values are from LL82, whereas the data for the disk type are from Fung (1984) (see also the appendix). The experimental relative occurrence of breakup types \( R \), is fitted as

\[
R_{f,50} = 4.18 \text{ CKE}_{50}^{-0.53}\left[1 + (D_S/D_L)^2\right] \quad \text{and} \tag{8}
\]

\[
R_{f,50} = 0.5\{1 - \exp[-1.63(W_s,50 - 1.3)]\} \quad \text{for} \tag{9a}
\]

\[
W_{s,50} \geq 1.3,
\]

where the Weber number \( W = \text{CKE}/S_T \).

\[
R_{r,50} = 0 \quad \text{for} \quad W_{s,50} < 0, \tag{9b}
\]

\[
R_{r,50} = 1 - (R_{f,50} + R_{s,50}) \quad \text{for} \quad R_{f,50} + R_{s,50} < 1, \quad \text{and} \tag{10a}
\]

\[
R_{d,50} = 0 \quad \text{for} \quad R_{f,50} + R_{s,50} \geq 1. \tag{10b}
\]

The condition \( R_{f,50} + R_{s,50} > 1 \) occasionally occurs because the equations for \( R_{f,50} \) and \( R_{s,50} \) are independent of each other. Both these values are proportionally reduced to sum to 1. When large drops collide at 50 kPa, more collisions involve filament and disk breakup. However, at 50 kPa, there are fewer filament breakpoints when the smaller drop diameter is close to the larger drop diameter and fewer disk breakpoints when the smaller drop is generally <0.1 cm in diameter.

For the large fragment diameters (suffix 3), the position of the peak for the Gaussian distribution is positioned at

\[
D_{f,50} = [D_{f,100}^3 + 4.90 \times 10^{-4}(\text{CKE}_{100} - 8.21)^{0.403} - 7 \times 10^{-4}]^{1/3}, \tag{11}
\]

\[
D_{s,50} = [D_{s,100}^2 + 2.17 \times 10^{-3}(\text{CKE}_{100} - 10.5)^{0.31} - 2 \times 10^{-3}]^{1/2}, \tag{12}
\]
\[ D_{d1,50} = (D_{d1,100}^3 + 4.3 \times 10^{-6} S_C^{2.2} - 1.044 \times 10^{-3})^{1/3}. \]

The 100-kPa diameters are based on Fung (1984). For the filament case, \( D_{f1,50} = D_{f1,100} \). Also, the term containing \( \text{CKE}_{100} = 8.21 \) was set to zero when \( \text{CKE}_{100} \leq 8.21 \) erg. When \( \text{CKE}_{100} \leq 10.5 \) erg, then the second term was omitted from the equation for the peak diameter of the sheet breakup Gaussian. Occasionally the resulting diameter was reset down to the coalescence diameter \( D_{\text{coal}} \). A similar adjustment was infrequently required for the calculation of the disk breakup Gaussian. For the remaining fragments, the 50-kPa probabilities at the modal diameters:

\[ P(F_{f1,50}) = \frac{F_{f1,50}}{F_{f1,100}} \left( \frac{F_{s,50}}{F_{s,100}} \right)^{1/2}, \quad \text{and} \quad P(F_{s,50}) = \frac{F_{s,50}}{F_{d,100}} \left( \frac{F_{s,100}}{F_{d,100}} \right)^{1/2}. \]

The subscripts \( f3 \) in Eq. (24) describes the probability that tiny filament fragments occur. The quantities \( \sigma \) and \( H \) are determined by iteration. In most cases the 50-kPa probabilities are the same as or lower than the 100-kPa values.

An example of a parameterization for a sheet is given in Fig. 1. The spread of the large fragment number distribution is comparable with the precision with which the data have been collected. The diameter of the coalesced drop is 0.19 cm, but there are a fair number of drops with diameters >0.19 cm.

3. Box models

Box models are used to study the evolution of raindrop spectra at 50 and 100 kPa in a square volume of atmosphere. Whatever falls out at the bottom of the box is reintroduced at the top. Forty logarithmically spaced bins distinguish between the size classes, and the drop mass is assumed to be doubling every second bin. The drop diameter range is from 53 \( \mu \)m to 5.6 mm. For each time step an equation is used to describe the change of drops with mass \( M_k \) through the interaction of the \( M_i \) and \( M_p \). The interaction is described by a coefficient matrix \( \mathbf{X}_{ijk} \). The change in mass is proportional to the time step \( \Delta t \). This leads to

\[ \mathbf{X}_{ijk} \text{ is a measure of the spread, } H \text{ is a constant indicative of height, and } \mu \text{ is the natural logarithm of the median value and is related to the modal diameter } D_{\text{mode}} \text{ by} \]

\[ \mu = \ln D_{\text{mode}} + \sigma^2. \]
The box model process is displayed in Fig. 2. It uses specifications for the interpretation of all the laboratory drop collision experiments by McTaggart-Cowan and List (1975), LL82, and Fung (1984). The higher bin range contains the largest drops used in the experiments whereas the lower end corresponds to the smallest drops (fragments) resolved by the photographic system. The resolution also affects the shape of the drop size distribution of the largest fragments in a breakup. Logarithmic spacing was chosen to increase the details at the lower end while keeping the number of bins manageable.

The coefficient matrix is given by

$$\Delta M_k = \sum_{i=1}^{40} \sum_{j=1}^{i} M_i M_j X_{ijk} \Delta t,$$

where $V$ in $X_{ijk}$ in (27) is a shape function describing the variation in mass distribution within a bin; $w$, $x$, and $y$ are the drop output, large drop input, and small drop input masses, respectively; and $K(w, x, y)$ is the “kernel.” Because the calculations are not sensitive to the shape function $V$, a constant mass concentration within the bin is used. This leads to a shape function $V(x) = 2(m_1 - m_2^2)$, where $m_i$ is the mass corresponding to the diameter at the lower end of the bin interval. The kernel is given by

$$K(m, x, y) = \{(1 - E_{coa}) P(m, x, y) + E_{coa} \delta(x + y - m) - \delta(m - x) - \delta(m - y) \} C(x, y),$$

where $E_{coa}$ is the coalescence efficiency, $P$ the fragment distribution rate, and $\delta$ the Dirac delta function. The fractional interaction rate is given by

$$C(x, y) = \frac{\pi}{4} (D_x + D_y)^2 \Delta V |E_{coll}|,$$

where $D_x$ and $D_y$ are the large and small drop diameters, respectively, $\Delta V$ is the difference in the drop terminal velocities, and $E_{coll}$ is the collection efficiency (assumed to be unity for the model). For the calculations of the kernel coefficients, the bins were divided into 12 logarithmic subintervals.

The products of the breakup process have been displayed in Part I. The smaller fragments in the filament, sheet, and disk breakups are described by lognormal distributions; Gaussians are used for the large fragments. For both pressure levels, five other kernels were developed: for coalescence, for all breakups together, and for filament, sheet, or disk breakup alone. This was done to determine the importance for mass transfer between any two diameters for any time step.

For the calculation of the kernel, the numerical technique is an extension of that by Gelbard and Seinfeld (1978). Simpson’s rule algorithms handled the tiny-fragment lognormals, whereas differences in error functions were used for the normally distributed larger fragments. It is emphasized that the pressures are contained in the kernel’s coefficients. When certain initial
spectra were used, it was at times necessary to decrease the size if the time step were less than the usual 1 s to avoid total depletion of any bin masses.

4. Equilibrium size distributions

In agreement with List (1988), all simulations of spectra evolutions for a given pressure lead to an equilibrium drop size distribution. This is illustrated by Figs. 3a,b with comparisons of number and concentrations per logarithmic diameter intervals for 50- and 100-kPa pressures. Note that it took 2 h of evolution to reach equilibrium. Lowering the pressure shifts the large drop mass peak from 1.7 to 2.0 mm, while the middle peak shifts to a smaller diameter. The middle peak is only visible as a shoulder for 100 kPa. For number concentration, the small drop peak is very visible and does not change with pressure. It is higher for low pressure, as is the case for the second peak. The higher peak for 1.9 mm at 100 kPa disappears for 50 kPa; it is only seen as a wiggle. In the mass distribution the decrease in mass around the large peak is compensated by a concentration increase at smaller diameters. The terms “small”, “mid-size,” and “large” drops refer to those of the peaks in the 100-kPa equilibrium. “Smallest” and “largest” drops refer to the limiting sizes of the box model: 53 μm and 5.6 mm, respectively.

Figure 4 indicates overall normalized changes in bin mass for the various interaction processes occurring at the 100- and 50-kPa equilibria. The initial spectrum for these calculations was MP50. Any other distribution would give the same result. The actual magnitudes of the normalized mass changes are directly proportional to the total water content and inversely proportional to the bin size. The general trends are in agreement with List and McFarquhar (1990) and Brown (1988). Figures 4a and 4b show that the small drops are depleted by coalescence and replenished by filament breakup. Sheet breakup controls the midsize drops (diameter ~0.7 mm) and adds to the largest ones (5 mm and bigger) at both pressures. With disk and filament breakup removing mass to a greater extent for the large drops, it is coalescence that replenishes the losses, resulting in a zero overall mass loss. The magnitude of the mass fluxes together with the small bin masses implies relatively short lifetimes for the large (diameter ~5 mm) drops. For 50-kPa disk breakup, very large drops add more to the large drops (Fig. 4b) than they do at 100 kPa.

Figures 5a and 5b provide the same information shown in Fig. 4, but they are bundled differently. Figure 5a underlines the similarity of the coalescence and breakup patterns. At sizes <~2 mm, breakup adds mass to every bin whereas coalescence removes drop mass. Interestingly, there are no net changes at a diameter of ~2 mm that are caused by any type of breakup. At diameters >~2 cm the roles between accretion and coalescence are reversed: coalescence leads to net mass growth whereas breakup removes water from the same categories. The role of the different types of breakup is depicted in Fig. 5b. Filament fragments are the main
mass sources for diameters <0.3 mm. Not much mass change occurs for drops with diameters 0.5 to 2 mm. Beyond 2 mm, filament breakup removes mass, more so at 50 than at 100 kPa. Note that at low pressure disk breakup moves more mass into the large drops at the low pressure. When the contribution of sheets diminishes, then sheet breakup contributes more (also at 100 kPa). At the position of the large peak not much net mass change occurs. For larger masses, the interplay of the processes indicates short bin lifetimes of the very large drops.

5. Evolution from a uniform number or mass spectrum

In running a model starting from a uniform mass distribution, time steps of 0.05 s were required to prevent

![Figure 4: Net mass change per bin mass for the equilibrium distributions at (a) 100 and (b) 50 kPa, for total results (all); filament, sheet, and disk breakups; and coalescence; "ll" refers to the LL82 parameterization (100 kPa) and "a5" to the 50-kPa parameterization described in section 2. Arrows indicate peaks in the 100-kPa equilibrium distribution.](image)

![Figure 5: Balancing the (a) coalescence and breakup and (b) relative importance of breakup types at 100 and 50 kPa; arrows indicate peaks in the 100-kPa equilibrium distribution.](image)
the mass in the largest drop bins from plummeting to zero and to allow a continuous decrease in subsequent time steps. Figures 6a and 6b document the evolution for the two pressures, 100 and 50 kPa. They show that the peaks developed very similarly within the same time for both pressures. Mass concentration changes are very insensitive to pressure. Astounding, however, is the time it takes to achieve equilibrium. This was first shown by Nissen et al. (2005) for rain rates, at the ground, of 5 mm h\(^{-1}\). Essentially, no spectra evolution toward an equilibrium distribution could be seen because the collision intervals were too long. Without drop interaction there is no spectrum evolution. This was one of the reasons to simulate reasonably heavy rain of 50 mm h\(^{-1}\).

The time evolution of the spectra at the two pressures is shown for running times of 1, 5, 20, and 45 min (Figs. 7a–d). Figure 7d shows that an elapsed time of 2700s is barely enough to reach equilibrium. Be aware of the changing ordinate scale.

Contoured values of mass fluxes, normalized by bin mass, are displayed in Figs. 8a–f for MP50 and for both pressures of 100 and 50 kPa. They are given for three categories: all processes, coalescence, and breakup. The point density is 40 across (one per bin) and one per minute in the time direction. The contours asymptotically parallel the time axis as equilibrium is approached. Comparisons for all processes show little difference in patterns except that the evolution is faster at the low pressure. This is also true for breakup and coalescence. At 50 kPa the maximum size for coalescence is \(\sim\)5 mm, whereas larger drops are allowed at ground level. The same is reflected in the parameterization of breakup.

The spectra evolution of the number concentration per logarithmic interval is shown for 100 and 50 kPa in Fig. 9. For both pressures the initial growth in drop population is concentrated in the 0.2–1.0-mm diameter range. A large fraction is due to filament breakup of larger drops. Most if the remaining growth is due to sheet breakup, especially for drops \(\sim\)0.7 mm. The “equilibrium” peaks (List 1988) at the smallest diameter become fairly distinct quite quickly, particularly at 100 kPa. However, the approach to equilibrium is quite different. At the higher pressure there is an overshooting in concentration, whereas the same peak develops gradually at 50 kPa. Higher collision rates at 100 kPa allow the lowest peak to be set in \(\sim\)20 min whereas it takes twice the time to establish at the lower pressure. This is also the case for the middle peak; the largest peaks take somewhat more time. These differences in patterns of the evolution of number concentration may represent the biggest effect of pressure change.

The formulation describing the peak in number concentration, often approximated by a Dirac delta function, is demonstrated by Fig. 10, originally presented by Nissen 1996. It gives the equilibrium distributions for two cases at 50 kPa. The difference between the two is that the Gaussians differ by a factor of 2 in height and a simultaneous factor of 0.5 in width. The decrease in height produces a clear three-peak distribution; doubling the height leads to a barely recognizable third peak. This reduced peak formulation was chosen for the processing of the 50-kPa information.

McFarquhar (2004) addressed this point and provided specific procedures of how to obtain optimal distributions while obeying mass conservation. This method was not applied here because the limited number of five cases might not have formed an adequate basis for meaningful statistics. The actual detailed stochastic breakup pattern with limited numbers of fragments per case would also have to be considered. In addition, the choice not to apply mass conservation in the LL82 case was a wise decision considering that the experiment
resolution was not sufficient to identify missing mass as belonging to the unresolved tiny fragments (K. Jellinghaus 2005, personal communication).

6. Summary and comments

The parameterization of drop interactions by LL82 for an air pressure of ~100 kPa has been used to adapt the description of the spectra evolutions in a consistent manner, be they mass or number concentration, to a pressure of 50 kPa. This allowed a study of the relationship between coalescence and breakup, as well as its individual filament, sheet, and disk breakup types. This then allowed comparisons of breakup at the two pressures. The evolutions of mass and number concentration spectra show the following trends:

1) The contributions to mass change at the two pressures are very similar throughout the drop size range. In general, the 50-kPa data show increased mass changes of coalescence and breakup compared to the 100-kPa parameterized experiments. This also applies to filament breakup; sheet breakup is not sensitive to pressure change. Disk breakup is a major producer of large fragments (>2 mm) at low pressure.

Fig. 7. Pressure dependence of spectra evolution from uniform MP50 for (a) 1, (b) 5, (c) 20, and (d) 45 min.
Fig. 8. Net changes in relative bin mass for MP50, for 100 and 50 kPa, for all processes, coalescence, and breakup. Dashed contours indicate negative values, contour interval is 0.001; contour values range from −0.012 to higher than 0.012.
2) The overall mass evolution is not noticeably pressure dependent. The evolution of the number concentration to equilibrium, however, is totally different. At 100 kPa the evolution starts with a rapid buildup and overshooting of the equilibrium peaks, whereas the peaks develop gradually at 50 kPa. Visually judged equilibria need twice the time for development at 50 kPa than at 100 kPa. Equilibrium distributions at 50 kPa do not show a large drop peak; there is a barely recognizable shoulder. However, changing the Gaussian to half the height and double the width recovers the large and middle drop equilibrium peaks. The need to use one or the other peak parameterization, however, is not clear. The experimental evidence on spectrum types is nonexistent because of lack of resolution. Thus, the approach used is similar to the previous parameterizations.

3) The calculations of concentrations for equilibrium number distributions require times of up to 12 h with 1-s time steps. For mass distributions the (single) peak still does not reach equilibrium within that time.

This leads to the question of importance of a development of a pressure-dependent parameterization of raindrop interactions covering the whole range of atmospheric conditions. Considerations include the following:

1) It is now obvious that the evolution of drop spectra is dependent on the frequency of drop interactions. Such frequencies may not be sufficiently high. At rain rates $R < 10 \text{ mm h}^{-1}$ there is no need to consider drop collisions with coalescence and breakup. For $R > 50 \text{ mm h}^{-1}$ there is definitely a need to apply it. Modeling of very heavy storms may gain when applying it.

2) Breakup is being described in four-dimensional parameter space. What about adding pressure as a fifth component, now that we have insight into two pressures? Is there a way to interpolate linearly between the two anchoring points at 100 and 50 kPa? That might be possible if a conformal transformation...
of one 4D surface into the other could be done. This is feasible when it comes to the distortion of objects, but this experience is more common for visual artists than for atmospheric scientists.

3) The examples developed in this paper used a box model for demonstration. However, more explicit modeling, first by one-dimensional shaft models, will establish that the drop spectra evolutions will be accelerated because there is a major growth component through accretion of cloud droplets. This may even overshadow drop growth by accretion of breakup fragments.

A numerical approach such as the one by Beheng et al. (2006) may provide answers more quickly than can be done by experiments followed by parameterizations. However, computer modeling has its own problems.

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APPENDIX

Fung's (1984) 100-kPa Equations Used in the 50-kPa Model

The following equations were not used in the 100-kPa box model but were incorporated in the 50-kPa model equations. CKE is collision kinetic energy [defined in Eq. (1)]. All constants are in cgs units.

The equation for the number of disk fragments [used in Eq. (7)] is

\[
F_{d,100} = 15 \left[ 1 + \text{erf} \left( \frac{\text{CKE} - 68}{22} \right) \right] + 2.33. \tag{A1}
\]

The equations for the peak positions of the 100-kPa diameters of the large fragments [used in Eqs. (11), (12), (13), and (14)] are for filament, sheet, and disk breakup respectively:

\[
D_{f1,100} = D_L - \frac{9.09 \times 10^{-6} \text{ CKE} + 5.56 \times 10^{-5}}{D_L^2}, \tag{A2}
\]

\[
D_{s1,100} = \left[ D_L^2 + D_S^2 - \frac{D_S}{D_L} (1.02 \times 10^{-3} \text{ CKE} + 0.004) \right]^{1/2}, \tag{A3}
\]

\[
D_{d1,100} = \left[ D_L^3 + D_S^3 - 2.35 \times 10^{-2} \left[ 1 + \text{erf} \left( \frac{\text{CKE} - 68}{22} \right) \right] - 0.001 \right]^{1/3}. \tag{A4}
\]

The 100-kPa peak position for the small fragment diameter from filament breakup [used in Eq. (14)] is given by

\[
D_{f2,100} = D_S + 3.29 \times 10^{-12} (\text{CKE} + 117)^{4.05} - 0.002. \tag{A5}
\]

REFERENCES


