

Geophysical Laboratory I, academic year: 2022/2023

FIRST STEPS TOWARDS CLOUD MICROPHYSICS MODELING

Agnieszka Makulska,
registration number: 417936

tutor: prof. dr hab. Hanna Pawłowska

date of submission: April 18, 2023
date of revision: May 18, 2023

1 Introduction

In this exercise an air parcel is considered, rising adiabatically with a constant velocity. Its evolution is assessed using an algorithm included in libcloudph++, a library for representing cloud microphysics in full numerical cloud models. A particle-based representation of cloud microphysics is used. The model is run with a given initial distribution of aerosol, with fixed initial conditions (such as temperature and pressure), but with different values of vertical velocity. Profiles of saturation, concentration of cloud droplets, mean volume cloud droplet radius and specific liquid water content are assessed. Profiles are calculated for different values of the time step of integration and the convergence of results is studied. The dependence of results on velocity is studied. The activation spectrum is assessed.

2 Parcel model

A 0-dimensional model of an air parcel, rising adiabatically with a constant velocity is used in this exercise. It is an idealized framework to study basic thermodynamical and microphysical properties of clouds, with a particle-based representation of microphysics. The particle-based scheme allows to track the properties of particles during the entire simulation. Each particle is characterised by its dry radius r_d and its wet radius r . Particles are represented by super-droplets. Each super-droplet represents a number of particles, with the same dry and wet radius and position. Microphysical processes are solved by an algorithm included in the libcloudph++ library. It is a library of algorithms for representing cloud microphysics in numerical cloud models, written in C++ [1]. Algorithms included in libcloudph++ are executed with the help of a simpler framework, written in Python.

The user specifies the initial temperature T_0 , the pressure p_0 , the water vapor mixing ratio r_{v0} of the parcel and parameters of the aerosol spectrum. The initial spectrum of wet radii is set to be in equilibrium with the environment, at initial T_0 , p_0 and r_{v0} . The parcel is then moved upwards with a constant velocity. Parameters of the model: the time step of integration, the maximum vertical displacement, the number of super-droplets used by the particle-based scheme and the number of substeps of condensation per each time step are also specified by the user.

The profile of pressure p is obtained by integrating the equation of hydrostatic balance:

$$\frac{dp}{dz} = -\rho g, \quad (1)$$

where z is the vertical displacement, ρ is the air density and g is the gravitational acceleration. The dry air density ρ_d at a given level is then calculated as a function of pressure, dry potential temperature and water vapor mixing ratio. Dry potential temperature and water vapor mixing ratio are variables which can only be changed due to microphysical processes. The condensational growth of droplets is solved with the particle-based scheme.

The model outputs the pressure, the temperature, the relative humidity, the water vapor mixing ratio and the dry potential temperature. The model also outputs moments of the particles size distribution. The i -th moment is defined as

$$m_i = \int_{r_{min}}^{r_{max}} r^i n(r) dr, \quad (2)$$

where r is the radius, n is the probability density function of concentration, r_{min} and r_{max} are left and right edges of the distribution. In the numerical model, instead of an integral, a sum is calculated over a number of bins specified by the user.

It is assumed that the distribution of atmospheric aerosol consists of lognormal modes. The hygroscopicity parameter κ is specified for each mode. A single lognormal mode is described by the equation:

$$n(r_d) = \frac{N_{tot}}{\sqrt{2\pi} r_d \ln \sigma} \exp\left(-\frac{(\ln r_d - \ln r_m)^2}{2 \ln^2 \sigma}\right), \quad (3)$$

where n is the probability density function of concentration, r_d is the dry radius, N_{tot} is the total concentration, σ is the geometric standard deviation, r_m is the mean dry radius of particles. Figure 1 shows an example of aerosol distribution with one lognormal mode.

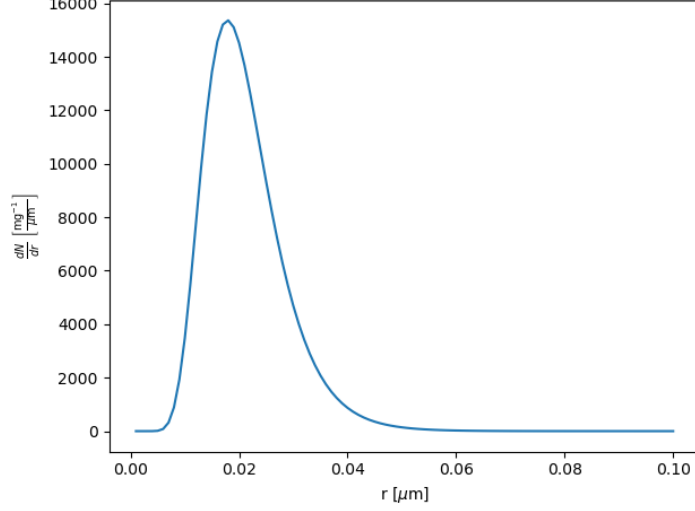


Figure 1: Probability density distribution of aerosol concentration, with one lognormal mode, with the average dry radius $r_m = 0.02 \mu\text{m}$, the geometric standard deviation $\sigma = 1.4$ and the total concentration $N_{tot} = 245 \frac{1}{\text{mg}}$.

3 Results

In the first part of the exercise the vertical velocity is set as constant. The model is run with different values of the integration time step. The influence of the time step on results is discussed.

The model is run with 1000 super-droplets, with vertical velocity 1 m/s. Hygroscopicity parameter is set to $\kappa = 1.28$. The model is run for 200 m. Initial conditions are: pressure $p_0 = 1013 \text{ hPa}$, temperature $T_0 = 300 \text{ K}$ and water vapor mixing ratio $r_{v0} = 0.022$, which corresponds to relative humidity $RH_0 = 0.983$. The distribution of aerosol is described by equation 3, with one lognormal mode, with average dry radius $r_m = 0.02 \mu\text{m}$, geometric standard deviation $\sigma = 1.4$ and total concentration $N_{tot} = 245 \frac{1}{\text{mg}}$.

Cloud droplets are defined as droplets, for which the radius exceeds their activation radius. Concentration of cloud droplets is calculated as the zeroth moment of the distribution of activated droplets. The mean volume radius is calculated as the third moment of the distribution of activated droplets, divided by its zeroth moment. Specific liquid water content q_c is calculated with the formula:

$$q_c = \frac{4}{3} \pi r_v^3 \rho_w N, \quad (4)$$

where N is the concentration of activated droplets, ρ_w is the density of water and r_v is the mean volume droplet radius.

Figure 2 shows vertical profiles of the concentration of cloud droplets, relative humidity, mean volume droplet radius and specific liquid water content, calculated with the parcel model.

$w=1.0$ m/s, $sd_conc=1000$, $\kappa=1.28$, $n_{aerosol}=245.0 \frac{1}{mg}$

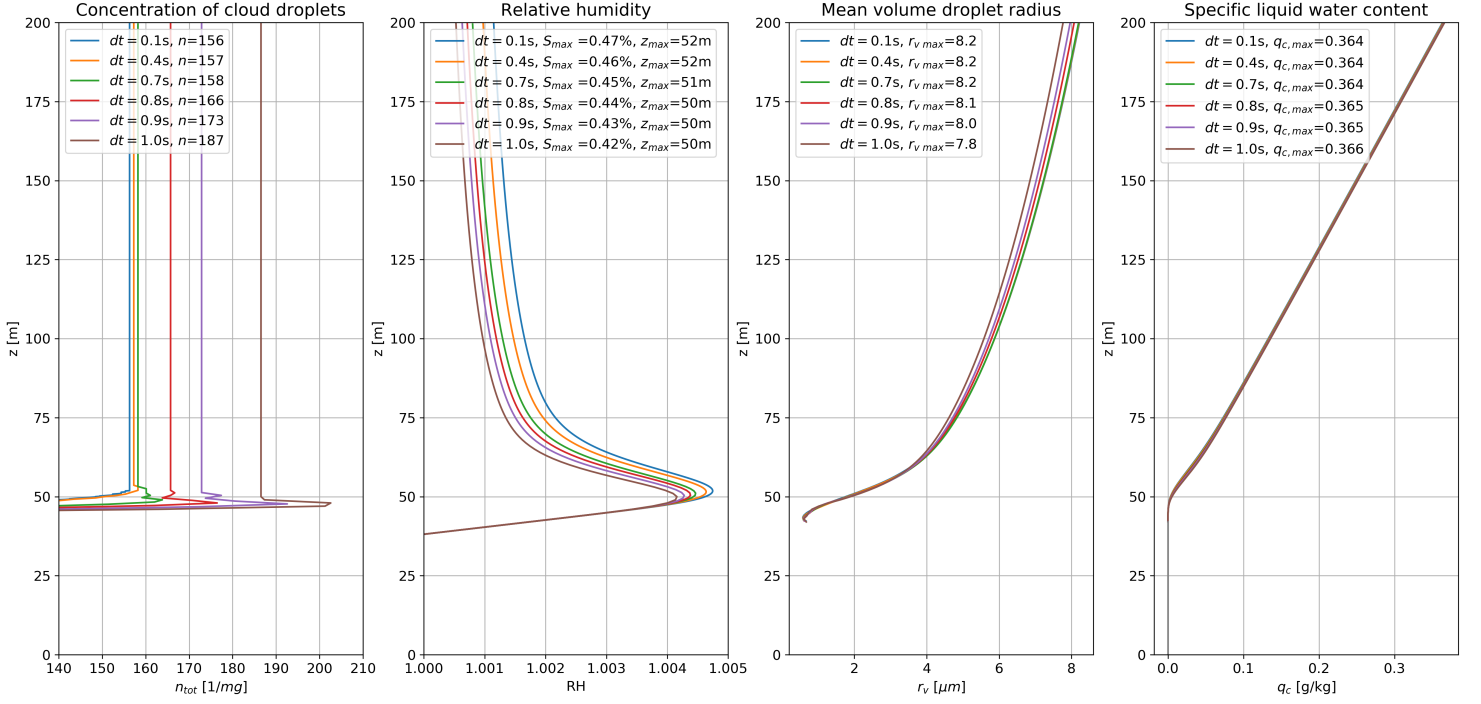


Figure 2: Profiles of the concentration of cloud droplets in 1/mg, relative humidity, mean volume droplet radius and specific liquid water content, calculated with 1000 super-droplets, with vertical velocity $v = 1$ m/s, hygroscopicity $\kappa=1.28$ and aerosol concentration $245 \frac{1}{mg}$. Different colors signify different values of the time step. Legends show the values of droplet concentration at the altitude 200 m (the first panel), maximum supersaturation and the height on which it occurs (the second panel), maximum mean volume droplet radius (the third panel) and maximum specific liquid water content (the fourth panel), for different time steps.

Figure 3 shows the same profiles as presented in figure 2, but limited to altitudes near the maximum of saturation.

$$w=1.0 \text{ m/s}, \text{sd_conc}=1000, \kappa=1.28, n_{\text{aerosol}}=245.0 \frac{1}{\text{mg}}$$

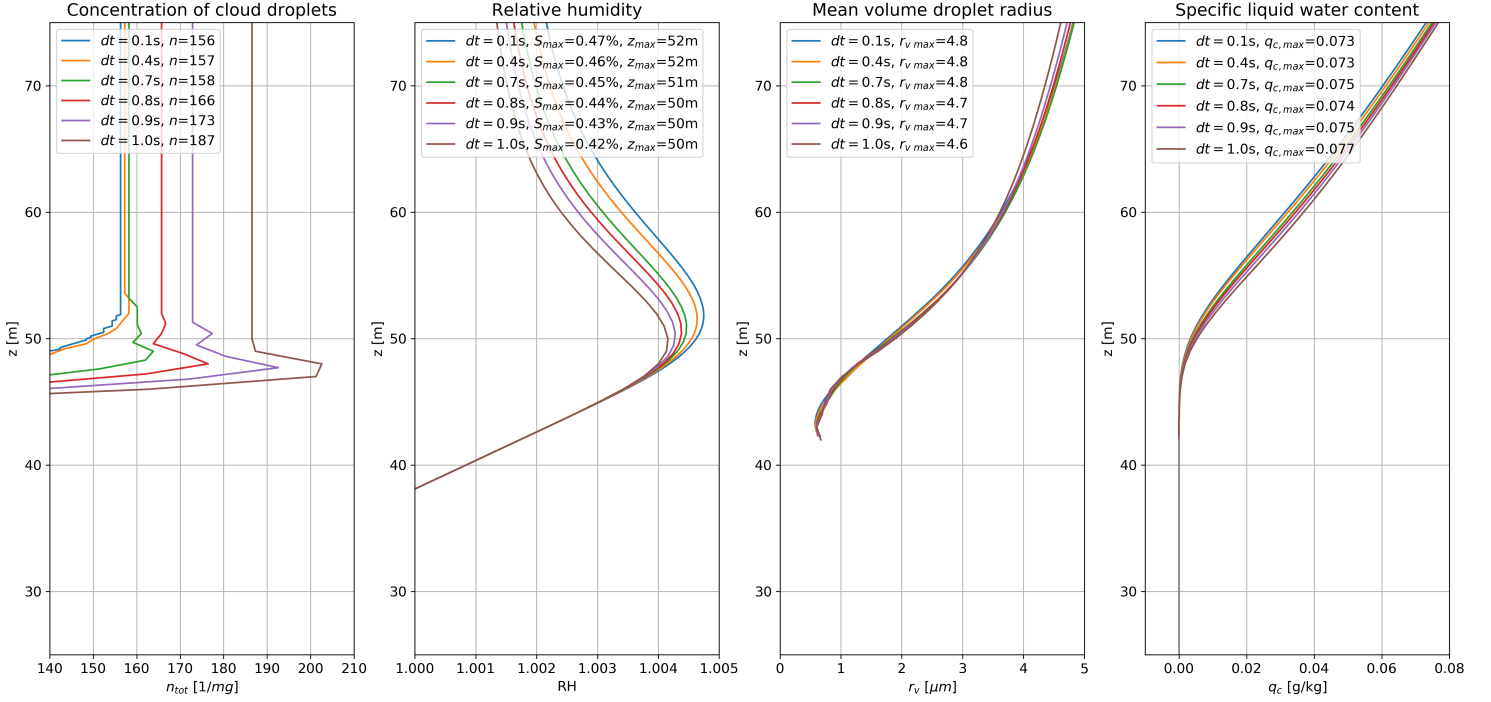


Figure 3: Profiles of the concentration of cloud droplets in 1/mg, relative humidity, mean volume droplet radius and specific liquid water content, limited to altitudes close to the maximum of saturation. Different colors signify different values of the time step. Legends show the values of droplet concentration at the altitude 75 m (the first panel), maximum supersaturation and the height on which it occurs (the second panel), maximum mean volume droplet radius (the third panel) and maximum specific liquid water content (the fourth panel), for different time steps.

For bigger time steps, the value of maximum saturation and the altitude at which it occurs are smaller, compared to small time steps. The value of maximum droplet concentration is larger for big time steps, compared to small time steps. Based on figures 2 and 3, it seems that the time step $dt = 0.1$ s is the most appropriate for the parcel model. For time steps larger than 0.1 s, there are significant jump discontinuities in profiles of cloud droplet concentration. Near the altitude of the maximum saturation, some droplets activate and later become deactivated, which can be seen in profiles of concentration. For all time steps except for $dt = 0.1$ s, the maximum value of cloud droplet concentration is reached on a lower altitude than the maximum saturation. This can be caused by the fact that for large time steps, the water vapor saturation is updated less frequently. When droplets grow, they absorb water vapor from the air, thus decreasing the relative humidity and limiting the growth of other droplets. If the time step is large, some droplets can grow without accurate information about the amount of water vapor in the air. Consequently, a droplet can cross the maximum of the Köhler curve and activate, even though in reality it should not.

For profiles of the mean volume droplet radius and specific liquid water content, results for different time steps do not vary significantly, and thus not all the lines can be distinguished in figures 2 and 3. Large droplets contribute the most to the value of the mean volume radius. Therefore, for large time steps such as $dt = 1$ s (when the smallest droplets are able to activate and concentration of activated droplets is larger compared to small time steps), the activation of small droplets doesn't have a significant influence on the mean volume radius. The specific liquid water content is limited, because the sum of the specific liquid water content and the specific humidity must be constant. The model is adiabatic, therefore the amount of liquid water in the cloud depends on thermodynamic properties at the cloud base, that are nearly the same for all time steps. Thus the specific liquid water content is nearly the same for all time steps. Similarly, the quantity $r_v^3 N$, where r_v is the mean volume droplet radius and

N is the concentration of cloud droplets, is nearly the same for all time steps. Concentrations N are different for different time steps, as well as values of r_v^3 , but the differences between r_v for different time steps are not very significant.

In the second part of the exercise, it is discussed how results of the model change, with the change of vertical velocity. Figure 4 shows the comparison of profiles of the concentration of cloud droplets, relative humidity, mean volume droplet radius and specific liquid water content, for different values of vertical velocity. The time step of integration is constant and equal to 0.1 s. The number of super-droplets is 1000 and hygroscopicity parameter κ is set to 1.28. Initial conditions are the same as in the first part of the exercise.

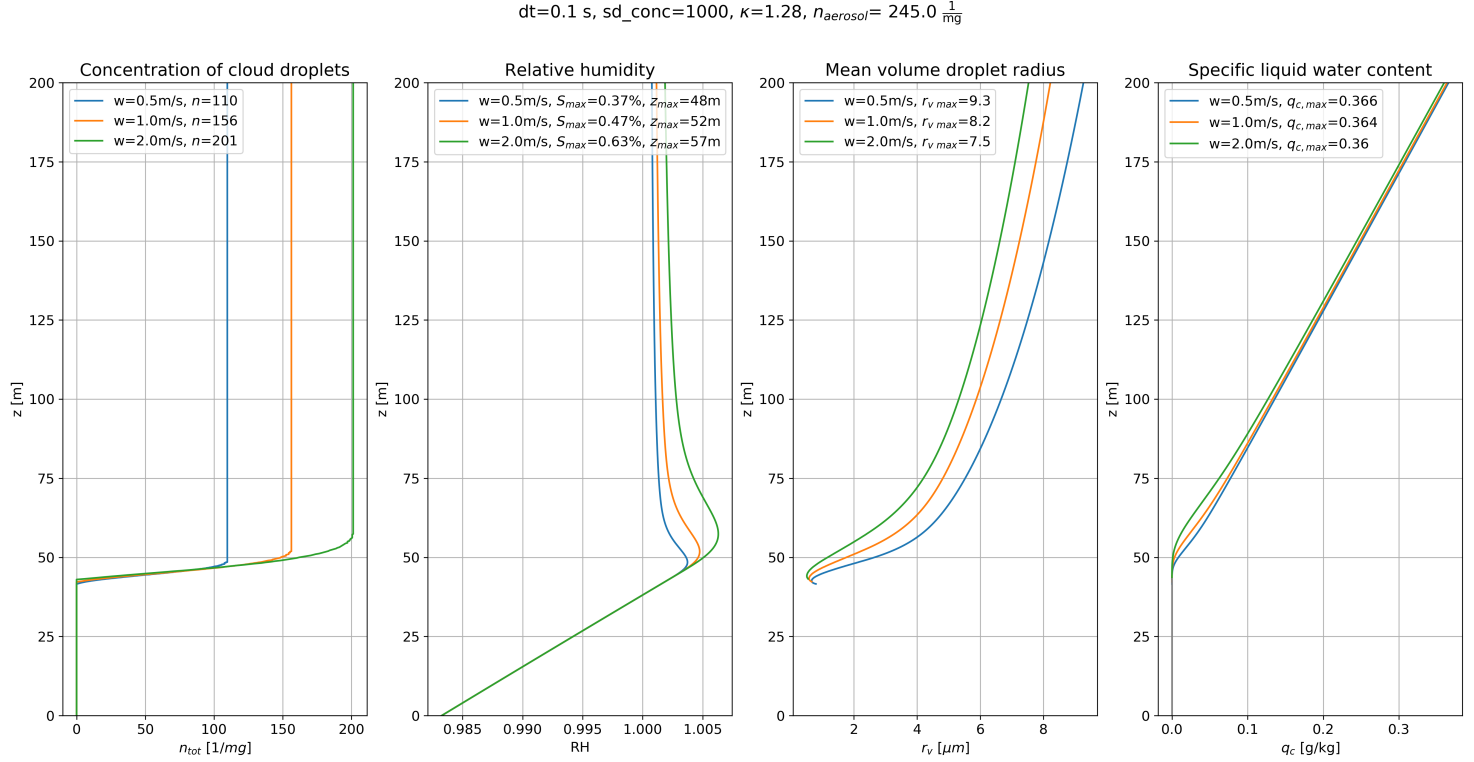


Figure 4: Profiles of the concentration of cloud droplets in 1/mg, relative humidity, mean volume droplet radius and specific liquid water content for different values of vertical velocity: 0.5 m/s, 1 m/s and 2 m/s. Legends show the values of droplet concentration at the altitude 200 m (the first panel), maximum supersaturation and the height on which it occurs (the second panel), maximum mean volume droplet radius (the third panel) and maximum specific liquid water content (the fourth panel), for different velocities.

As the velocity increases, the value of maximum saturation increases. This can lead to the fact, that more droplets are able to activate, and thus the total concentration of cloud droplets is larger for large velocities, compared to small velocities. However, the liquid water content in the air is limited, as the sum of specific liquid water content and specific humidity must remain constant. Specific liquid water contents for different velocities do not vary significantly. This means, that as the total number of droplets increases with an increase of velocity, their mean volume radius must decrease, which can be seen in figure 4. It is also true for the results shown in figures 2 and 3, but there differences in concentrations are smaller than in the case of figure 4.

One of the goals of the exercise is to study the convergence of results, depending on the integration time step. Figure 5 shows the total concentration of activated droplets at the end of a parcel simulation, depending on the integration time step. Results are presented for different values of vertical velocity.

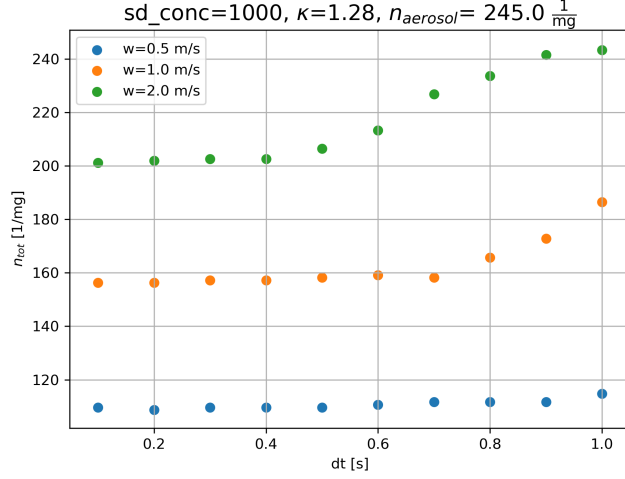


Figure 5: The total concentration of activated droplets depending on the integration time step. Different colors indicate different vertical velocities. The number of super-droplets is 1000, hygroscopicity parameter κ is 1.28 and the initial aerosol concentration is $245 \frac{1}{\text{mg}}$.

The total concentration of activated droplets increases with the increase of the time step. It can result from the fact, that for large time steps, water vapor saturation is not updated frequently enough. Some droplets can activate before the saturation is updated and remain activated, even though in reality they would not. As the time step becomes small, the concentration of activated droplets approaches a constant value. For small time steps (between 0.1 s and 0.4 s), values of the concentration are roughly constant for each velocity. The concentration of activated droplets increases also with the increase of vertical velocity. It can be explained by the fact, that for large velocities, the maximum saturation is larger and thus more droplets are able to activate, compared to small velocities, as can be seen in figure 4.

Cloud droplets are defined as activated droplets (droplets for which the wet radius exceeds their activation radius). A formula for the total number of activated droplets can be found. The equilibrium saturation S_{eq} over a droplet is described by the Köhler curve:

$$S_{eq}(r, \kappa, r_d, T) = \frac{r^3 - r_d^3}{r^3 - r_d^3(1 - \kappa)} \exp\left(\frac{A(T)}{r}\right), \quad (5)$$

where r is the wet radius, r_d is the dry radius, κ is the hygroscopicity parameter, $A(T)$ is a parameter which depends on the temperature: $A(T) = 2\sigma/(\rho_l R_v T)$, where $\sigma = 75.64 \times 10^{-3}$ is the surface tension, ρ_l is the density of water, R_v is the specific gas constant for water vapor and T is the temperature. Figure 6 shows Köhler curves with fixed hygroscopicity parameter and temperature, but for different values of the dry radius.

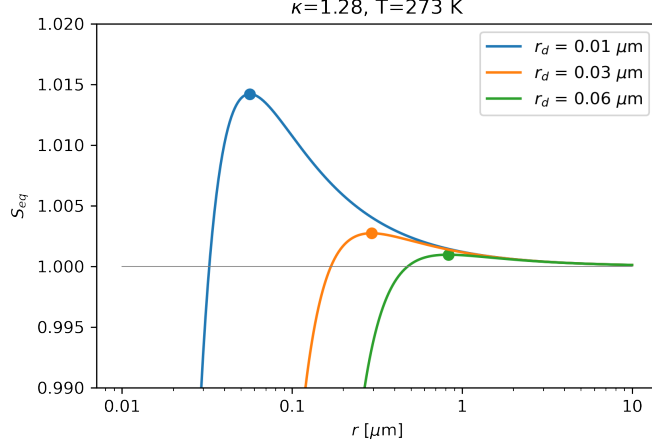


Figure 6: Köhler curves for different values of dry radius r_d , with hygroscopicity parameter $\kappa = 1.28$ and temperature $T = 273$ K. Maxima of Köhler curves are marked with dots.

The wet radius and the equilibrium saturation at the maximum of the Köhler curve are defined as activation radius and activation saturation. Figure 6 shows, that the activation saturation over a droplet decreases with the increase of its dry radius. One can introduce a critical dry radius, r_{cr} . It is the dry radius of a droplet, which in a given saturation is activated (the saturation is equal to the activation saturation at the maximum of the Köhler curve corresponding to the dry radius). The critical dry radius r_{cr} corresponds to the activation saturation S^* . From the Köhler curve, one can derive the relation between the critical dry radius and the activation saturation:

$$r_{cr} = \left(\frac{4A(T)^3}{27\kappa(S^* - 1)^2} \right)^{1/3}. \quad (6)$$

Droplets with dry radii larger than r_{cr} are activated in saturations smaller than S^* , because the activation saturation decreases with the increase of the dry radius. An expression for the total concentration N of droplets with dry radii larger than r_{cr} is an integral of equation 3, from r_{cr} to infinity:

$$N(r_{cr}) = \int_{r_{cr}}^{\infty} n(r_d) dr_d = \frac{N_{tot}}{2} \left(1 + \operatorname{erf} \left(\frac{\ln(r_m/r_{cr})}{\sqrt{2} \ln \sigma} \right) \right), \quad (7)$$

where erf is the error function. By substituting r_{cr} from equation 6 to equation 7, one obtains a formula for the total concentration of droplets which are activated in saturations smaller or equal S^* . This is a formula for the activation spectrum - the total concentration of activated droplets, expressed as a function of the saturation.

Figure 7 shows the activation spectrum, calculated with the parcel model. For each value of saturation, it shows the concentration of droplets for which activation saturation is smaller than the actual saturation. Results are presented for different values of the integration time step. In addition, theoretical results are shown, calculated with equation 7.

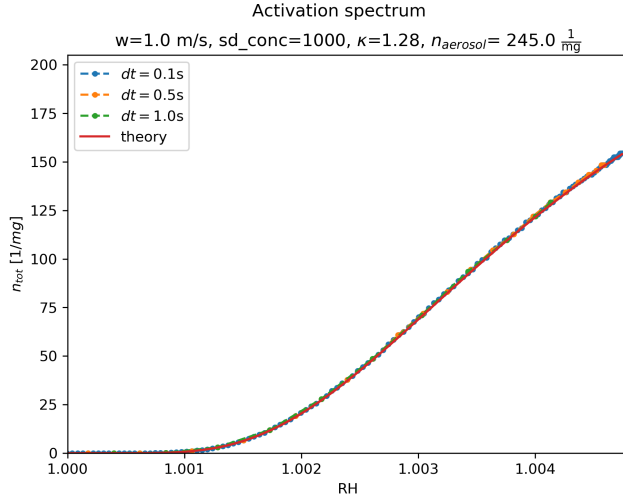


Figure 7: Activation spectrum calculated with the parcel model, for different values of the time step: 0.1 s (blue line), 0.5 s (orange line) and 1 s (green line). Theoretical formula of the activation spectrum is presented (red line).

Activation spectrum calculated with the parcel model agrees with theoretical results, for all values of the integration time step.

4 Conclusions

The evolution of an air parcel, rising adiabatically with a constant velocity was assessed, using an algorithm included in the libcloudph++ library. The model was run with fixed initial conditions and a fixed distribution of aerosol, but with different values of vertical velocity and different integration time steps.

Profiles of saturation, concentration of cloud droplets, mean volume droplet radius and specific liquid water content were assessed with a constant value of vertical velocity, but for multiple values of the integration time step. It was found that saturation and droplet concentration depend significantly on the value of the time step. Specific liquid water content and mean volume droplet radius are roughly the same for all values of the time step. It was concluded, that the time step 0.1 s is the most appropriate for the parcel model. It was also concluded, that for large time steps, some droplets can be activated even though in reality they would not, because the model does not update the saturation of water vapor frequently enough. The relation between the integration time step and the concentration of activated droplets was studied. It was concluded, that the concentration increases with the increase of the time step, but for sufficiently small time steps it approaches a constant value, for each value of the vertical velocity.

Profiles of saturation, concentration of cloud droplets, mean volume droplet radius and specific liquid water content were assessed with a constant value of the integration time step, but with different values of vertical velocity. There are significant differences between cloud droplet concentration, water vapor saturation and mean volume droplet radius, calculated with different vertical velocities. As the velocity of the updraft increases, the maximum water vapor saturation increases. Thus, more droplets can activate and their mean radius decreases, as the specific liquid water content is roughly the same for all velocities.

Activation spectrum was assessed and compared with theoretical results. It was found that activation spectrum calculated with the parcel model agrees with theoretical results, for all values of the integration time step.

References

- [1] Arabas S., Jaruga A., Pawlowska H., and 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, vol. 8, pp. 1677-1707, doi: 10.5194/gmd-8-1677-2015

- [2] Petters, M. D. and Kreidenweis, S. M.: A single parameter representation of hygroscopic growth and cloud condensation nucleus activity, *Atmos. Chem. Phys.*, 7, 1961–1971, doi:10.5194/acp-7-1961-2007, 2007.
- [3] *Cloud-microphysics modelling group at the Institute of Geophysics, Faculty of Physics, University of Warsaw - GitHub webpage*