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Basics of numerical convergence in cloud microphysics modeling

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1 Introduction

An air parcel rising adiabatically with a constant velocity is considered. Its evolution is assessed using an algorithm included in libcloudph++ library. It is a library for representing cloud microphysics, which can be used for different numerical cloud models, including the parcel model. Simulations are performed with different values of the time step of integration and different numbers of substeps for condensation. The goal of the exercise is to determine the time step of integration and the number of substeps for condensation required for the convergence of the model. Two different aerosol size distributions are used, one of which corresponds to the distribution in a culumus cloud, and the other corresponds to the distribution in a stratocumulus cloud. Simulations are run with different values of vertical velocity. It is discussed how the required time step of integration depends on the initial distribution of aerosol and on the vertical velocity.

2 Parcel model

A 0-dimensional model of an air parcel that rises adiabatically with a constant velocity is considered. 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 characterized 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 libcloudph++, 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.

Modeling the evolution of cloud droplets involves finding numerical solutions to a set of differential equations. Accuracy of results increases with decreasing time step of the method. An equation that requires short time steps is the equation for condensational growth of droplets. The goal of the exercise is to determine the time step required for the convergence of the growth equation in the model of a raising parcel. The required time step may depend on details of the modeled case, such as the aerosol size distribution or the vertical velocity of the parcel.

In the parcel model, the initial parameters are: the temperature T_0, the pressure p_0, the water vapor mixing ratio r_{v0} and parameters of the aerosol distribution. The initial spectrum of wet radii is set to be in equilibrium with the environment, at the initial T_0, p_0 and r_{v0}. The parcel is then moved upward with a constant velocity. The number of super-droplets used by the particle-based scheme and the time step of integration are specified by the user. The number of substeps for condensation per each time step is also specified, which allows to solve the equation of condensational growth with a greater precision. The profile of pressure p is obtained by integrating the hydrostatic balance equation:

$$\frac{dp}{dz} = -\rho g, \tag{1}$$

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 calculated as a function of pressure, dry potential temperature, and the mixing ratio of water vapor. The dry potential temperature and the mixing ratio of water vapor are variables that can only be changed due to microphysical processes. The condensational growth of droplets is solved with the particle-based scheme.

It is assumed that the size 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:

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

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.

In the exercise, two different distributions of dry particles are considered, one of which corresponds to the distribution in cumulus clouds and the other corresponds to the distribution in stratocumulus clouds. The distributions are presented in figures 1 and 2. On average, stratocumulus clouds consist of particles with smaller dry radii, than cumulus clouds.

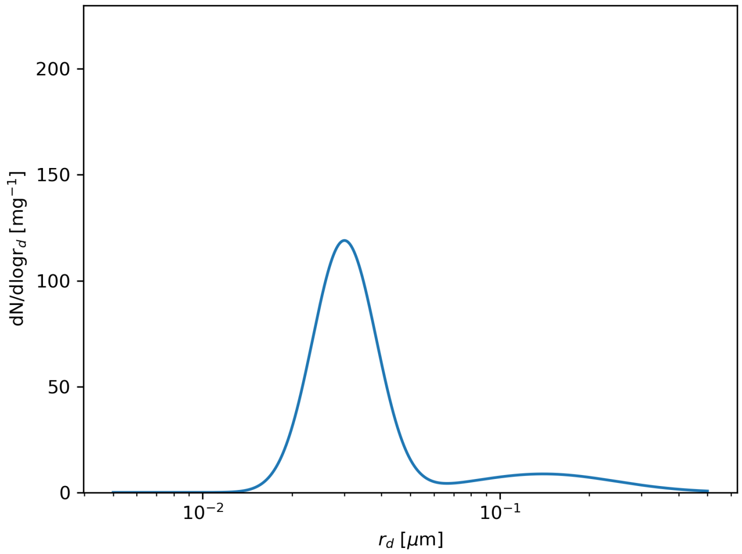

Figure 1: The distribution of dry particles, which corresponds to a cumulus cloud. The distribution has two lognormal modes, one with parameters $r_m = 0.03$ μm, $\sigma = 1.28$, $N_{tot} = 73.5 \frac{1}{\mathrm{mg}}$ and the other with parameters $r_m = 0.14$ μm, $\sigma = 1.75$, $N_{tot} = 12.25 \frac{1}{\mathrm{mg}}$. For both modes the hygroscopicity is κ=0.61.

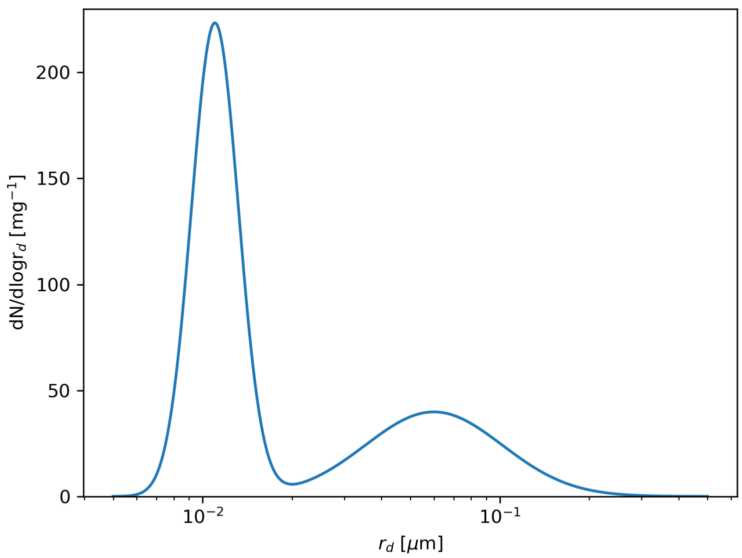

Figure 2: The distribution of dry particles, which corresponds to a stratocumulus cloud. The distribution has two lognormal modes, one with parameters $r_m = 0.011$ μm, $\sigma = 1.2$, $N_{tot} = 102 \frac{1}{\mathrm{mg}}$ and the other with parameters $r_m = 0.06$ μm, $\sigma = 1.7$, $N_{tot} = 53 \frac{1}{\mathrm{mg}}$. For both modes the hygroscopicity is κ=0.61.

3 Results

The parcel model is run with 1000 super-droplets, with the vertical velocity 2 m/s. Initial conditions are: pressure $p_0 = 1013$ hPa, temperature $T_0 = 300$ K and water vapor mixing ratio $r_{v0} = 0.022$, which corresponds to the relative humidity $\mathrm{RH}_0 = 0.983$. Figures 3 and 4 show results of the parcel model, with the distribution of dry particles corresponding to cumulus and stratocumulus clouds respectively, for different time steps of integration. There are no substeps for condensation.

Figures 3 and 4 show the concentration of cloud droplets in 1/mg, the relative humidity, the mean volume droplet radius and the specific liquid water content. Cloud droplets are defined as droplets having a wet radius that exceeds their activation radius. Different colors correspond to different values of the integration time step.

Figures 5 and 6 show results of the parcel model, with aerosol distributions corresponding to cumulus and stratocumulus clouds respectively, for different numbers of substeps for condensation. The time step of integration is equal to 1 s.

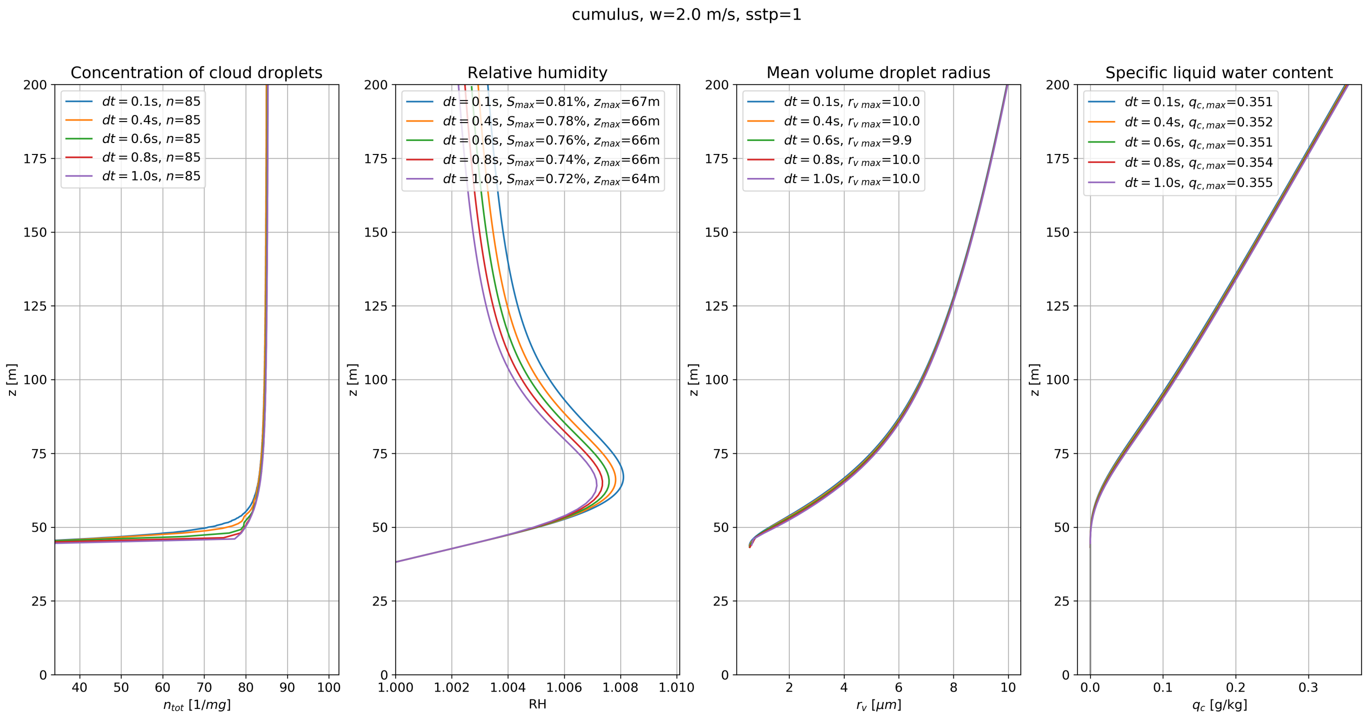

Figure 3: Results of the parcel model with the aerosol distribution corresponding to cumulus clouds and vertical velocity 2 m/s, with different integration time steps, but no substeps for condensation. Legends show values of the droplet concentration at the altitude 200 m, the maximum supersaturation and the height on which it occurs, the maximum mean volume droplet radius and the maximum specific liquid water content.

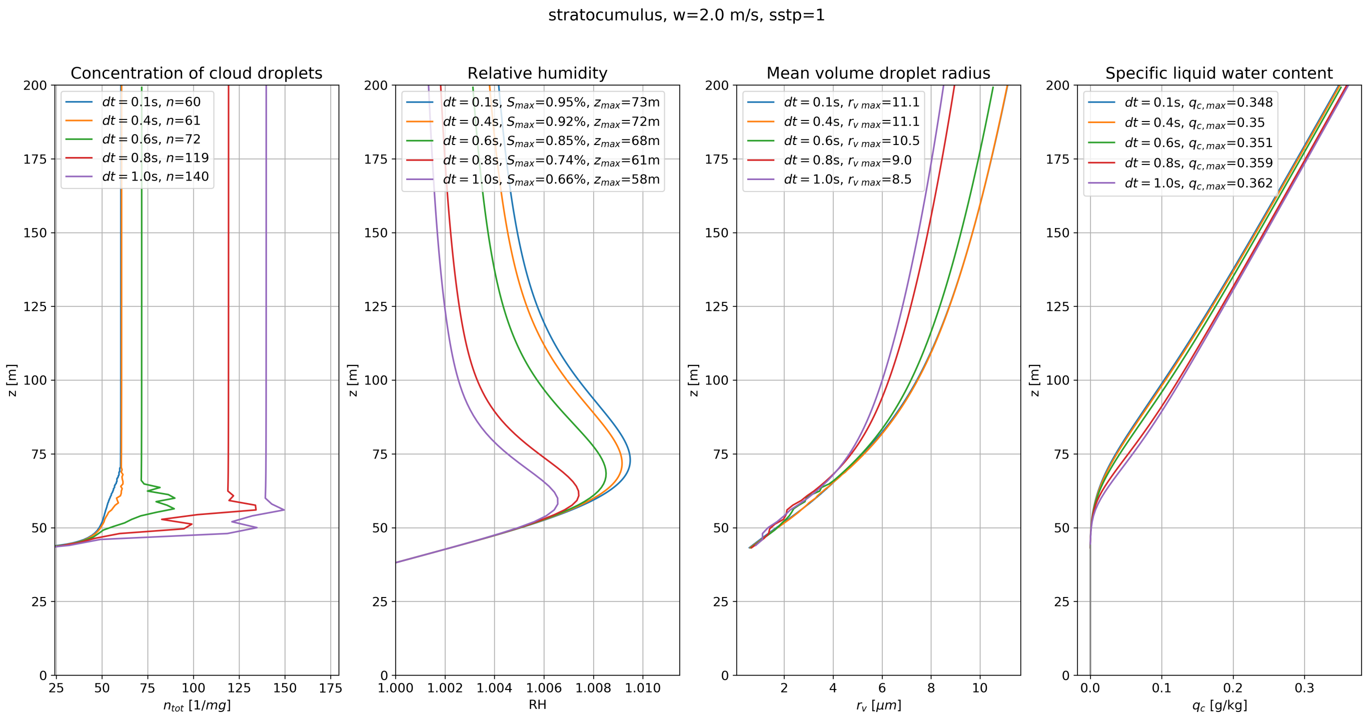

Figure 4: Results of the parcel model with the aerosol distribution corresponding to stratocumulus clouds and vertical velocity 2 m/s, with different integration time steps, but no substeps for condensation. Legends show selected values of the profiles, the same as in figure 3.

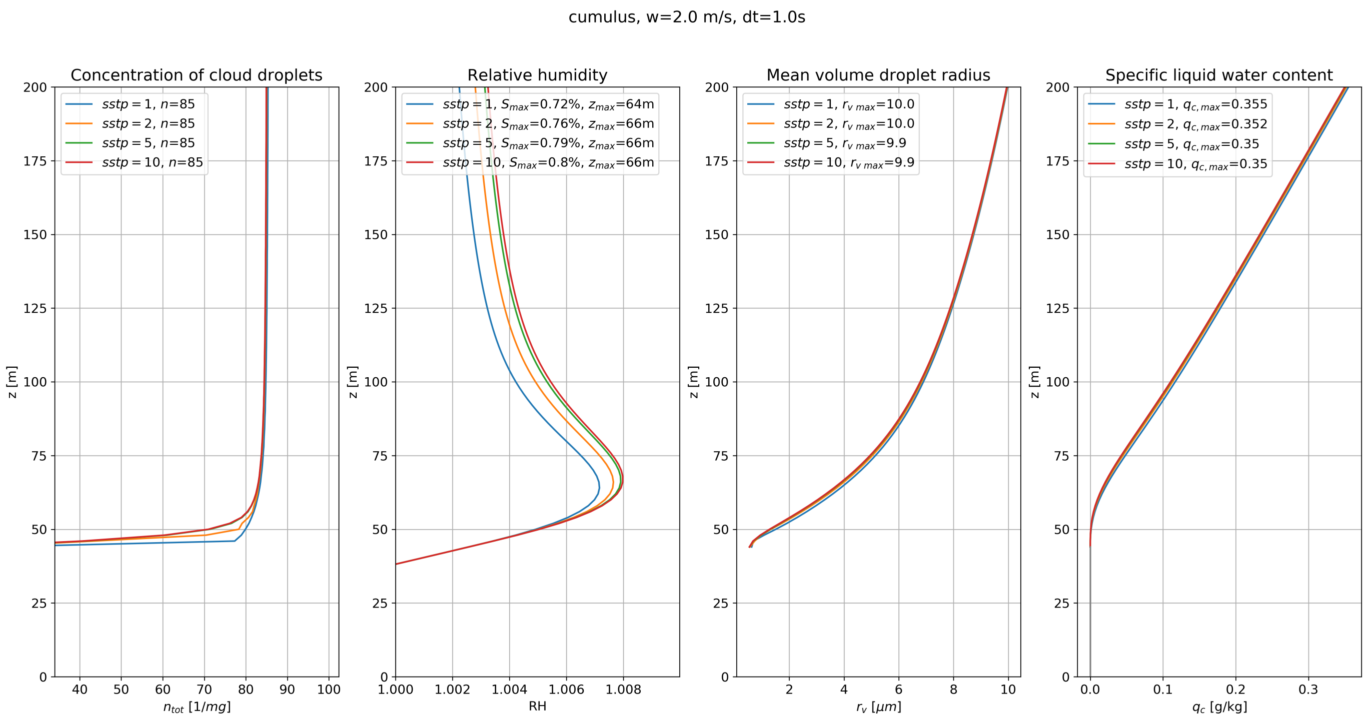

Figure 5: Results of the parcel model with the aerosol distribution corresponding to cumulus clouds and vertical velocity 2 m/s, with the integration time step 1 s, but with different numbers of substeps for condensation ($sstp$). Legends show selected values of the profiles, the same as in figure 3.

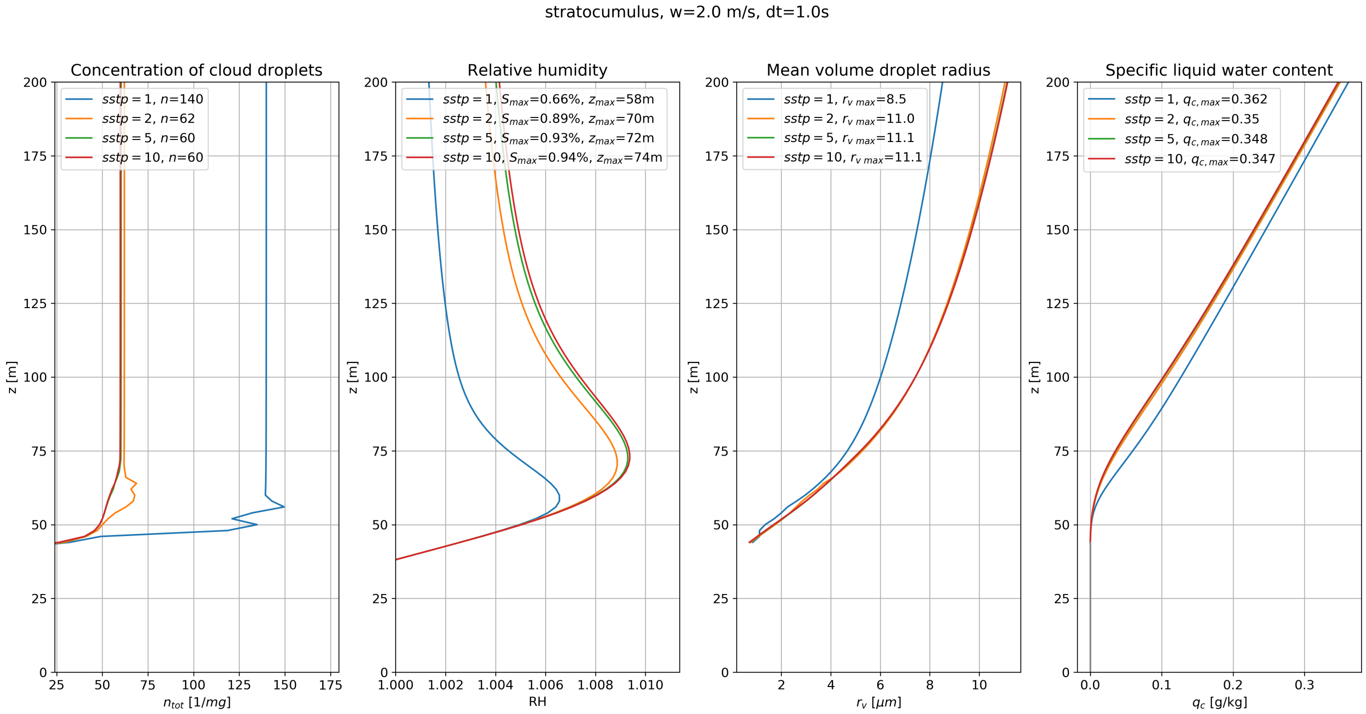

Figure 6: Results of the parcel model with the aerosol distribution corresponding to stratocumulus clouds and vertical velocity 2 m/s, with the integration time step 1 s, but different numbers of substeps for condensation ($sstp$). Legends show selected values of the profiles, the same as in figure 3.

The results obtained with the distribution of aerosol corresponding to cumulus clouds do not vary significantly with the time step of integration or with the number of substeps for condensation. For large time steps, the maximum of relative humidity is slightly lower, compared to the short time steps. Similarly, for a small number of substeps, the maximum of relative humidity is slightly lower, compared to simulations with a large number of substeps.

The results obtained with the distribution of aerosol corresponding to stratocumulus depend significantly on the time step of integration and on the number of substeps for condensation. For large time steps, the concentration of activated droplets is much larger compared to that for small time steps. The maximum of relative humidity and the altitude at which it occurs are smaller for large time steps, compared to that for small time steps. For large time steps, near the altitude of maximum saturation, some droplets activate and later become deactivated, which can be seen in profiles of concentration. The mean volume droplet radius varies significantly depending on the time step. The specific liquid water content varies slightly depending on the time step. Similarly, for simulations with the time step 1 s, results of the model vary significantly depending on the number of substeps for condensation.

Figures 7 and 8 show the total concentration of activated droplets at the end of the parcel simulation (at the altitude of 200 m), depending on the time step of integration and on the velocity, with aerosol distribution corresponding to cumulus and stratocumulus clouds respectively. There are no substeps for condensation.

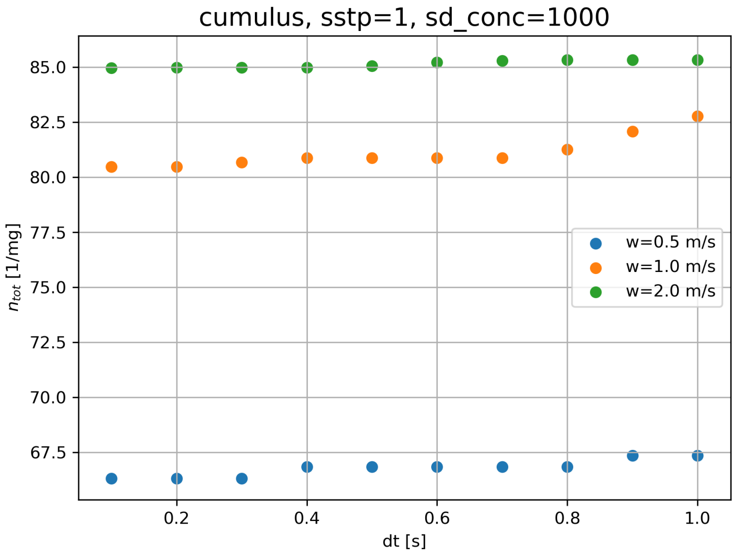

Figure 7: The total concentration of activated droplets depending on the integration time step, with no substeps for condensation, with the aerosol distribution corresponding to cumulus clouds. Different colors indicate different vertical velocities.

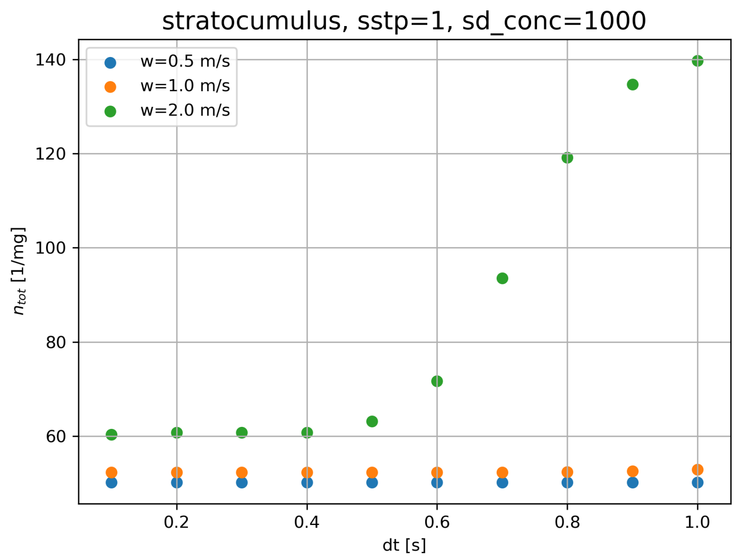

Figure 8: The total concentration of activated droplets depending on the integration time step, with no substeps for condensation, with the aerosol distribution corresponding to stratocumulus clouds. Different colors indicate different vertical velocities.

Figures 9 and 10 show the total concentration of activated droplets at the end of the parcel simulation (at the altitude of 200 m), depending on the number of substeps for condensation and on the velocity, with aerosol distribution corresponding to cumulus and stratocumulus clouds respectively. The integration time step is equal to 1 s.

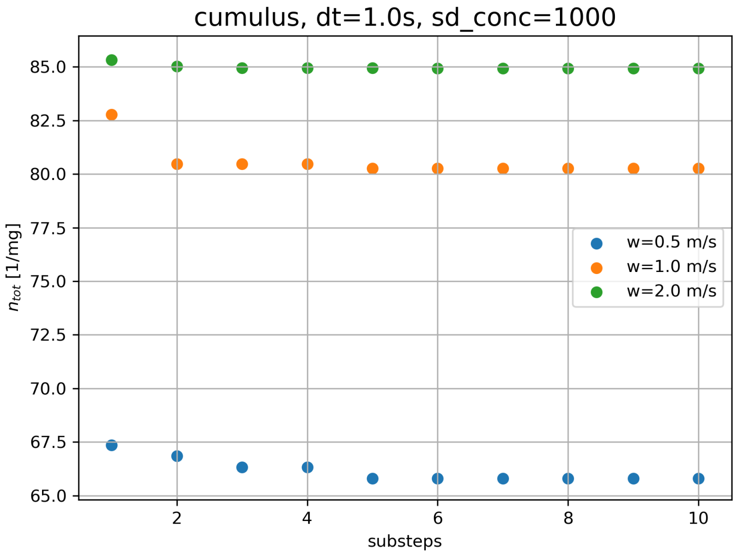

Figure 9: The total concentration of activated droplets depending on the number of substeps for condensation, with the integration time step 1 s, with the aerosol distribution corresponding to cumulus clouds. Different colors indicate different vertical velocities.

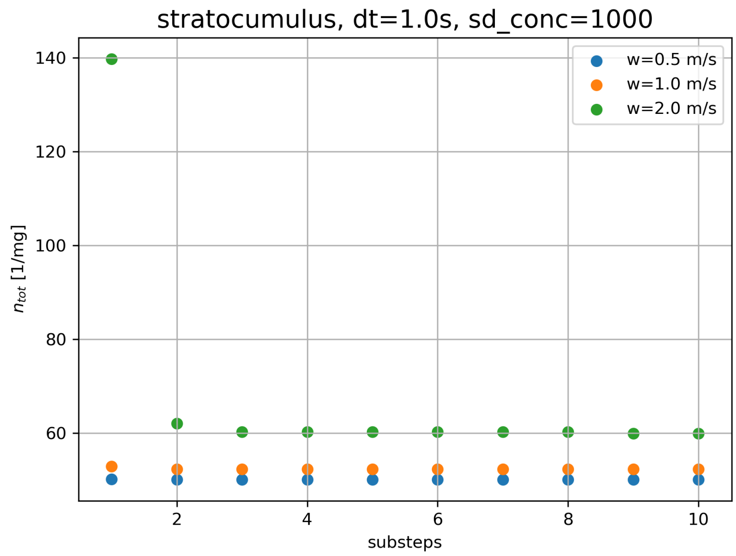

Figure 10: The total concentration of activated droplets depending on the number of substeps for condensation, with the integration time step 1 s, with the aerosol distribution corresponding to stratocumulus clouds. Different colors indicate different vertical velocities.

For simulations in which the distribution of aerosol corresponds to that in cumulus clouds, the concentration of activated droplets does not depend significantly neither on the integration time step nor on the number of substeps for condensation. Results are similar for all of the time steps considered. The concentration of activated droplets increases slightly for time steps greater than 0.8 s. In the case where the time step is 1 s, the concentration of activated droplets is slightly higher for simulations in which there are no additional substeps for condensation, compared to simulations with more than one substep for condensation. However, in general, for simulations in which the aerosol distribution corresponds to cumulus, each of the time steps can be considered appropriate.

For simulations in which the aerosol distribution corresponds to that in stratocumulus clouds, the concentration of activated droplets depends significantly on the integration time step, as well as on the number of substeps for condensation. In the case where the vertical velocity is 2 m/s, the concentration of activated droplets grows rapidly for integration time steps greater than 0.5 s. Thus, the required time step is 0.5 s or smaller. In the case where the time step is 1 s, the required number of substeps for condensation is 2 or more. However, the required time step also depends on the velocity. For simulations with vertical velocities 0.5 m/s and 1 m/s, the results are similar for all time steps, and thus each time step can be considered appropriate.

The concentration of activated droplets depends significantly on the velocity of the updraft. For simulations with large velocities, the concentration of activated droplets is larger, compared to simulations with small velocities. It results from the fact that the value of maximum saturation is larger in updrafts with larger velocities, and thus more droplets are able to activate, compared to updrafts with smaller velocities.

The sharp increase in the concentration of activated droplets, for the aerosol distribution corresponding to stratocumulus, with vertical velocity 2 m/s can be explained by the activation of droplets from the smaller mode of the distribution. Figures 11 and 12 show the distribution of wet radii for stratocumulus. Results are presented for the altitude $z = 35$ m (where the relative humidity is roughly equal to 1) and for the altitude $z = 200$ m (at the end of the parcel simulation). The distribution of wet radii is presented separately for the range 0.01-7 μm and for the range 7-12 μm.

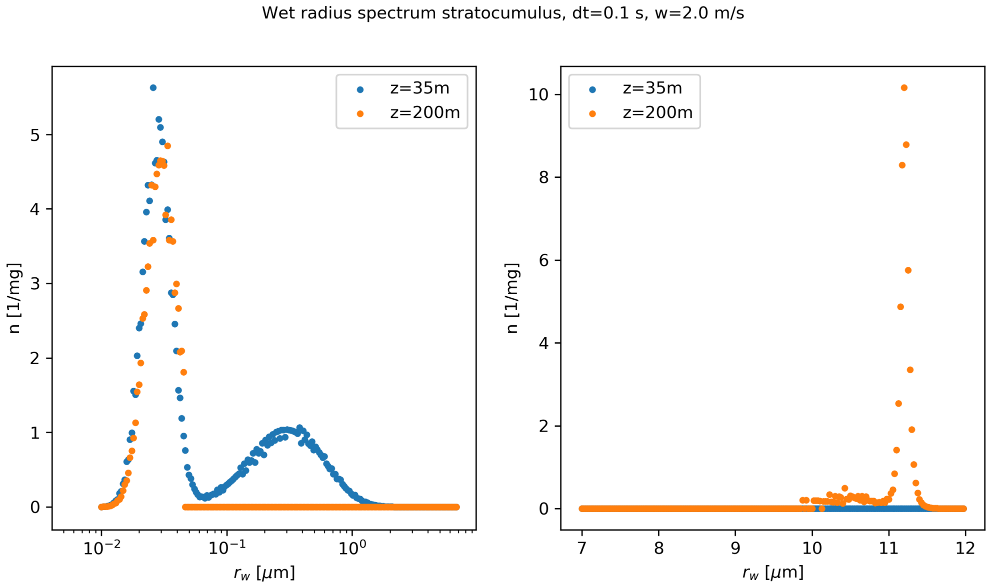

Figure 11: The distribution of wet radii for stratocumulus at the the altitude $z = 35$ m and at the the altitude $z = 200$ m. The simulation is run with the integration time step 0.1 s. The distribution of wet radii is presented separately for the range 0.01-7 μm (the left panel) and for the range 7-12 μm (the right panel).

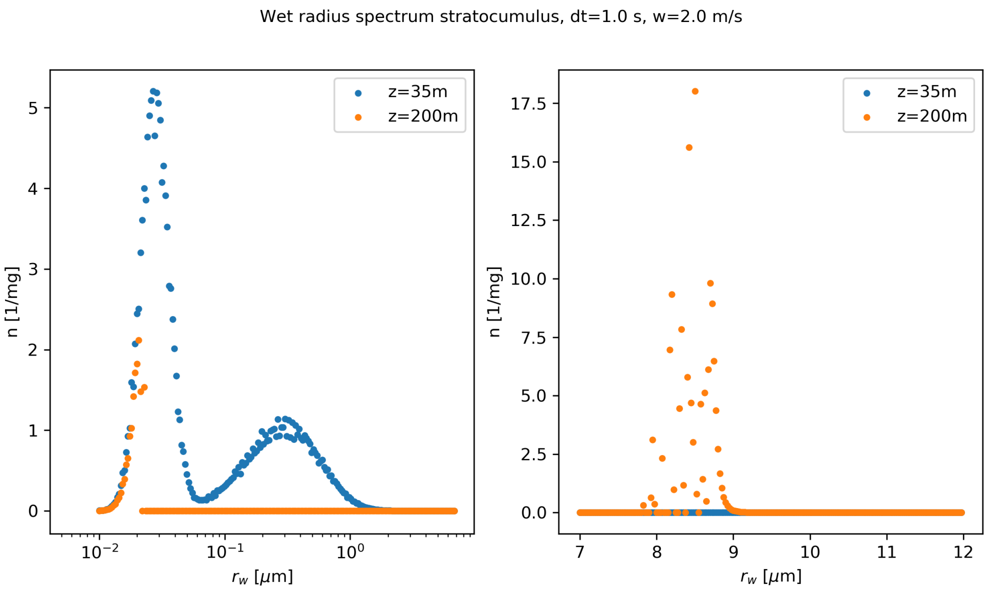

Figure 12: The distribution of wet radii for stratocumulus at the the altitude $z = 35$ m and at the the altitude $z = 200$ m. The simulation is run with the integration time step 1 s. The distribution of wet radii is presented separately for the range 0.01-7 μm (the left panel) and for the range 7-12 μm (the right panel).

In the case where the time step is equal to 0.1 s, many particles remain in the range of wet radii between 0.01 μm and 0.05 μm, corresponding to one of the initial modes of distribution, indicating that particles in this mode are mostly not activated. However, in the case where the time step is equal to 1 s, at the altitude of 200 m there are very few particles with wet radii between 0.01 μm and 0.05 μm, which means that almost all particles from this mode of distribution have been activated. Thus, using the large time step of 1 s results in the activation of droplets from the smaller mode of distribution (with smaller dry radii), which does not happen in the case where the time step is 0.1 s. This can be caused by the fact that for larger time steps, the relative humidity is updated less frequently. When droplets grow, they absorb water vapor from the air, thus decreasing the relative humidity and limiting the growth of all droplets. For larger time steps, when the relative humidity is updated less frequently, some droplets can cross the maximum of the Köhler curve and activate before the saturation is updated. Such droplets can remain activated in the model, although in reality they would not.

Figures 13 and 14 show the distribution of wet radii for cumulus, for the simulation with vertical velocity 2 m/s. Results are presented for the altitude $z = 35$ m (where the relative humidity is roughly equal to 1) and for the altitude $z = 200$ m (at the end of the parcel simulation). The distribution of wet radii is presented separately for the range 0.01-9 μm and for the range 9-11 μm.

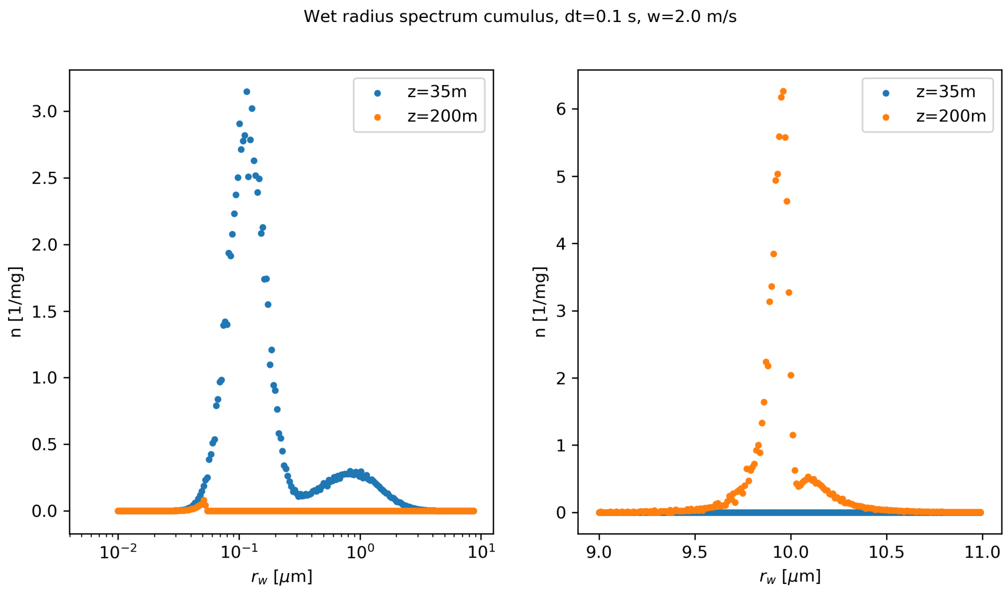

Figure 13: The distribution of wet radii for cumulus at the the altitude $z = 35$ m and at the the altitude $z = 200$ m. The simulation is run with the integration time step 0.1 s. The distribution of wet radii is presented separately for the range 0.01-9 μm (the left panel) and for the range 9-11 μm (the right panel).

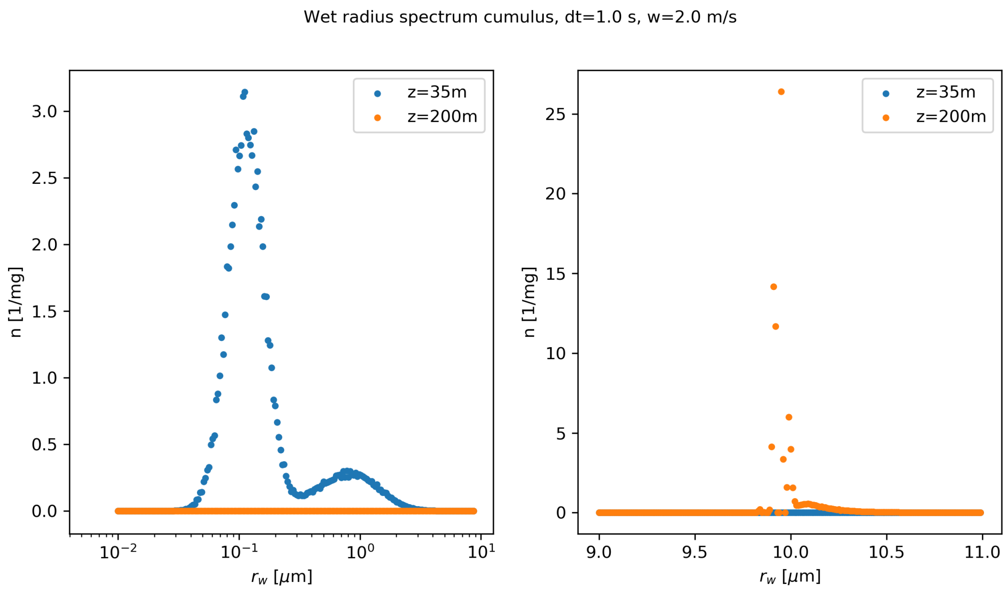

Figure 14: The distribution of wet radii for cumulus at the the altitude $z = 35$ m and at the the altitude $z = 200$ m. The simulation is run with the integration time step 1 s. The distribution of wet radii is presented separately for the range 0.01-9 μm (the left panel) and for the range 9-11 μm (the right panel).

For cumulus, in the case where the time step is 0.1 s, almost all particles are activated at the height $z = 200$ m, only the smallest particles remain unactivated. In the case where the time step is 1 s, all particles are activated at the height $z = 200$ m. Thus, for cumulus there is almost no difference between the concentration of activated particles in simulations with different time steps.

In general, it can be concluded that simulations for stratocumulus clouds (which correspond to aerosol size distribution with smaller dry radii, compared to cumulus) demand a smaller time step of integration or a larger number of substeps for condensation, compared to simulations for cumulus clouds.

4 Conclusions

The evolution of an air parcel, rising adiabatically with a constant velocity, was assessed using an algorithm included in the libcloudph++ library. Simulations were performed with different time steps of integration and different numbers of substeps for condensation. Two distributions of dry particles were considered, one corresponding to cumulus clouds and the other corresponding to stratocumulus clouds. It was found that for simulations in which the distribution of aerosol corresponds to cumulus clouds, the results do not depend significantly neither on the integration time step nor on the number of substeps for condensation. For simulations in which the aerosol distribution corresponds to stratocumulus clouds, the time step required for the convergence of the model depends on the velocity. In the case where the vertical velocity is 2 m/s, the concentration of activated droplets increases sharply for time steps greater than 0.5 s. It is a result of the activation of particles from one of the modes of particle distribution, which do not activate with smaller time steps. However, in cases where the vertical velocity is 0.5 m/s or 1 m/s, results of the model do not depend significantly on the time step. In general, the required time step and the required number of substeps for condensation depend on the aerosol size distribution and on the vertical velocity of the parcel.

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] *Cloud-microphysics modelling group at the Institute of Geophysics, Faculty of Physics, University of Warsaw - GitHub webpage*