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A study of aerosol activation at the cloud edge with high resolution numerical simulations

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ABSTRACT

High resolution numerical simulations are used to study the structure of the cloud edge area. We consider an aerosol distribution function with a similar aerosol core size (12 nm). The aerosol composition is assumed to be water soluble NaCl. Depending on the specific conditions in the investigated cloud edge area, water is evaporated or activated from the aerosol surface. We use a publicly available high order domain code for direct numerical simulation (DNS) in combination with the Smagorinsky subgrid scale model. We compare 2D and 3D model results of turbulent air motion of aerosol particles with varying grid cell sizes. We show that a 2D model with high resolution gives a more realistic number of activated particles than the corresponding 3D model with lower resolution. We also study the effects of aerosol dynamics on turbulent fields and show that water vapor condensation and evaporation have significant effects on temperature and supersaturation fields.

1. Introduction

Atmospheric aerosol particles affect the Earth's radiative balance both by scattering solar radiation and by acting as cloud condensation nuclei (CCN). CCN are a subset of all the particles that are able to form cloud droplets in atmospheric conditions. The radiative properties of clouds depend on the number of cloud droplets, and an increase in CCN concentration increases the cloud droplet number concentration (CDNC) (Twomey, 1977). A global decrease in CCN by year 2100, resulting from decreased sulfur dioxide emissions, could decrease CDNC by 20% (Makkonen et al., 2012). The change in CDNC, together with decreasing aerosol direct effect due to a decrease in aerosol concentration, would change the aerosol total forcing from present day to year 2100 by up to 1.4 W m^{-2} (Makkonen et al., 2012).

CDNC does not depend on the activation at cloud base in any simple manner, but the cloud is a dynamic system with spatially and temporally varying properties. More cloud droplets may form due to in-cloud activation, and entrainment of air from cloud edges may lead to formation of fresh cloud droplets (Brenguier and Grabowski, 1993; Wyszogrodzki et al., 2011; Slawinska et al., 2012). On the other hand, mixing at cloud boundaries, or in-cloud dynamics, can cause part of droplets to evaporate (Wood et al., 2002; Romakkaniemi et al., 2009; Morales et al., 2011).

In-cloud dynamics can be important especially in stratus type clouds with long in-cloud residence time of air parcels. Mixing at cloud boundaries takes place in all clouds, and the type of mixing depends on the conditions and mixing time scales. In homogeneous mixing, all droplets lose water but their number concentration is not affected. In heterogeneous mixing, a fraction of the droplet population experiences evaporation and forms aerosol particles with size much smaller than the size of prevailing cloud droplets. Depending on the time scales, the moisture content of entraining air, and the size of droplets, either homogeneous or heterogeneous mixing can be dominating (Andrejczuk et al., 2009).

Different phenomena related to aerosol cloud interactions and cloud dynamics involve a large range of scales. Microphysics of cloud–aerosol interactions can be studied by process models,

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or so called box models, which are mainly used to study how and which aerosol particles are able to form cloud droplets. At the other end of the scale are global models, which are needed to assess how changes in cloud properties affect the global radiation budget. Between these scales there are cloud resolving model (CRM) or large eddy simulation (LES) model that can be used to study cloud dynamics and for example the effect of aerosol on drizzle formation. However, even in CRM the scale (resolution > 1 m) is such that subgrid-scale turbulence needs to be parameterized. One of the methods to provide these parameterizations is direct numerical simulation (DNS) which can be used to study for example cloud boundaries up to a scale of few meters, or few tens of meters (e.g. (Mellado, 2010; Lanotte et al., 2009; Kumar et al., 2013)).

In previous studies, direct numerical simulations have been used to model microscale cloud–clear air mixing (Andrejczuk et al., 2004, 2006). The model physics was based on the Boussinesq approximation: density, kinematic viscosity, and the molecular diffusivity of the temperature and water vapor are assumed to be constant. The temperature evolution is determined by the thermal flux and by the release/absorption of the energy due to evaporation/condensation of/on water droplets. Additionally, they ignore the solute effect (Seinfeld and Pandis, 2006) and consider 16 size classes of the cloud droplets, with droplet sizes linearly distributed from 0.78 to 24 μm.

Comparing these earlier studies on aerosol cloud formation processes with the new model in this paper, the most important differences are: the gas is compressible; thermal conductivity and diffusion coefficients of every species and of a mixture are not constant and are described by the accurate expressions (Babkovskaia et al., 2011); thermal flux, change of energy by evaporation/condensation and viscous heating are included in the energy equation; and the solute effect is taken into account. To study the activation of aerosol particles we take 80 classes of the cloud droplets with the droplet size logarithmically distributed from 80 nm to 10 μm. We take the grid sizes of 0.5 cm, 1 cm, 2 cm, and 4 cm. Since the considered grid sizes are larger than the estimated Kolmogorov scale of $O(1)$ mm, we use the Smagorinsky subgrid scale model with parameter $C_s = 0.15$ for turbulent viscosity (Andrejczuk et al., 2004; Haugen and Brandenburg, 2006).

This paper is organized as follows. A detailed description of the model is presented in Section 2. Section 3.1 presents a 1D model to study aerosol evaporation/condensation (further we use *aerosol dynamics*) in a cloud edge area in a laminar regime. Sections 3.2–3.4 present results from 2D and 3D models with different resolutions. The main objective of this study is two-fold: to test the importance of the model resolution and to compare 2D and 3D model runs for correct simulations of aerosol activation. In Section 3.5 we study the effect of turbulent motion on aerosol dynamics. In Section 4 we will provide our conclusions.

2. Methods

We use the open source PENCIL code, which implements a high order finite difference method for compressible hydrodynamic flows. The code is highly modular and comes with a large selection of physics modules. It is widely documented in the literature and has been used for many different applications ((Dobler et al., 2006; The PENCIL Code, 2001), and references therein). Recently, a detailed chemistry module has been implemented, including an accurate description of all necessary quantities, such as diffusion coefficients, thermal conductivity, and reaction rates (Babkovskaia et al., 2011). This module was well tested by using a commercial code (Chemkin) for calculations of a turbulent combustion process. Our new aerosol module, coupled to the PENCIL Code, is now prepared for calculating condensation dynamics of aerosol particles. In the simulations, the composition of the aerosol cores is assumed to be NaCl which is a soluble aerosol and will dilute inside the droplets.

Originally, the PENCIL Code was developed for studying turbulent motions, so it is well suited for modeling the fluid mechanical processes in atmospheric clouds. Additionally, due to an accurate description of the chemistry, the PENCIL Code is a powerful tool for studying the aerosol dynamics in a turbulent medium with complicated chemical composition. The scientific goal for the construction of the new model is to investigate the spatial distribution of aerosol particles, turbulent mixing of clouds with the environment and the influence of turbulence on aerosol dynamics (and vice versa).

2.1. Fluid dynamic equations

The continuity equation is solved in the form

$$\frac{\mathrm{D}\ln\rho}{\mathrm{D}t} = -\nabla\cdot\boldsymbol{U}, \tag{1}$$

where $\mathrm{D}/\mathrm{D}t = \partial/\partial t + \boldsymbol{U}\cdot\nabla$ is the advective derivative, ρ is density, and $\boldsymbol{U}$ is velocity.

The momentum equation is written in the form

$$\frac{\mathrm{D}\boldsymbol{U}}{\mathrm{D}t} = \frac{1}{\rho}(-\nabla p + \boldsymbol{F}_{\mathrm{vis}}) + \boldsymbol{k}B, \tag{2}$$

where p is pressure, $\boldsymbol{k}$ is the unit vector in the vertical, B is buoyancy, and

$$\boldsymbol{F}_{\mathrm{vis}} = \nabla\cdot(2\rho\nu_t\boldsymbol{S}) \tag{3}$$

is the viscous force, where $\boldsymbol{S}_{ij} = \frac{1}{2}\left(\partial\boldsymbol{U}_i/\partial x_j + \partial\boldsymbol{U}_j/\partial x_i\right) - \frac{1}{3}\delta_{ij}\nabla\cdot\boldsymbol{U}$ is the traceless rate of strain tensor, and ν_t is turbulent viscosity. Following Haugen and Brandenburg (2006), in Smagorinsky model we use $\nu_t = (C_s\Delta)^2\sqrt{2\boldsymbol{S}^2}$, where Δ is the filter size which is equivalent to the mesh size.

The equation for the mass fractions of each species (except water vapor) is

$$\rho\frac{\mathrm{D}Y_k}{\mathrm{D}t} = -\nabla\cdot\boldsymbol{J}_k, \tag{4}$$

where $Y_k = \rho_k/\rho$ is the mass fraction, ρ_k is the density of kth component, and $\boldsymbol{J}_k$ is the diffusive flux for species k. For water vapor we have

$$\rho\frac{\mathrm{D}Y_{wk}}{\mathrm{D}t} = -\nabla\cdot\boldsymbol{J}_{wk} - \rho C_d, \tag{5}$$

where C_d is the condensation rate.