Abstract

Thermodynamic processes in the atmosphere shape the weather and climate of a given area. These processes are influenced by many factors such as orography, vicinity of water bodies, ocean currents, land use, and the presence of clouds. The role of clouds in the Earth's atmosphere system extends over a wide range of temporal and spatial scales. The quantitative description of such multi-scale phenomena is a challenging research task. To address this complex problem, special experimental facilities and advanced modeling techniques are required. Knowledge in this area is essential for the development of improved numerical models for weather and climate forecasting. For that reason, cloud microphysical effects, including those related to droplet–droplet and droplet–air interactions, are of particular interest. However, these small-scale processes, that determine the collision rate and hence precipitation formation, cannot be resolved in the mesoscale numerical weather prediction (NWP) models. This results from the huge disparity between the horizontal resolution of contemporary NWP models, $\mathcal{O}(1 \text{ km})$, and the typical sizes of cloud droplets, $\mathcal{O}(10 \text{ µm})$. Therefore, the processes at unresolved scales can only be represented in a statistical manner by employing the so-called parametrizations which are the main source of uncertainty in numerical weather forecasts.

Developing realistic parametrizations requires an accurate description of the small-scale atmospheric processes. To quantify these phenomena, a suitable numerical tool is needed. In recent decades, direct numerical simulations (DNS) have been widely established as a useful approach to resolve the flow structures down to the finest (Kolmogorov) scales. When combined with Lagrangian particle tracking (LPT) and a point-particle approximation, the method enables accurate tracking of large numbers of droplets in turbulence. Additionally, the droplet–droplet aerodynamic interaction (AI) can be taken into account via superimposing Stokes disturbances of neighboring droplets, leading to the so-called hybrid DNS (HDNS). While HDNS accurately represents long-range AI among the droplets, it fails to account for the strong short-range lubrication forces. Accordingly, one of the primary goals of this study is to improve AI representation of HDNS by additionally considering lubrication effects. The original proposed approach for treating AI is then used to compute collision statistics of dispersed droplet systems in homogeneous isotropic turbulence. The statistics include the collision kernel (rate), average radial relative velocity (RRV) between droplets, and radial distribution function (RDF) which is a measure of spatial clustering. The results show that, in the absence of gravity, inclusion of the lubrication effect reduces the RRV and collision kernel, but enhances the RDF (clustering) at the droplet scale.

The computational performance of this massively parallel implementation of HDNS, with the innovative method for treating AI, has been assessed by measuring the wall-clock time of major numerical operations. It has been observed that the computational time increases not only with the number and size of the particles, but also with the size of the lubrication region.

Moreover, simulations in larger domains showed an improvement in the performance when using a greater number of processors. These data are useful in planning future numerical experiments, particularly those with meshes of higher resolutions.

Following the investigations on the improvements in the representation of AI, the focus was directed towards two other aspects related to the short-range lubrication forces. The first one concerns non-continuum effects in the air flow between droplets when the separation distance in the gap is comparable to the mean free path of the air molecules. The second aspect addresses the viscous internal circulations of water inside the droplets induced by the tangential stress acting on their surfaces. In this approach, droplets are treated as non-deformable spherical fluid particles that have mobile interfaces with the surrounding flow of air. Either assumption results in a lower drag when the droplets approach, thereby enhancing collision rate. To evaluate the difference between these models, gravitational collision efficiency of a pair of water droplets settling in still air has been computed. Each effect leads to a larger collision efficiency; however, the non-continuum lubrication exhibits a stronger enhancement compared to the fluid drop model. Furthermore, the results show that at higher inertia of larger droplets, the importance of the non-continuum lubrication or internal water circulation diminishes compared to the effects of inertia. These results provide a preliminary understanding for the impact of AI representation on the dynamics of collision, paving the way for utilizing these models in systems of droplets interacting in turbulence.

Accordingly, the next analyzed problem concerns the influence of different AI models on the collision statistics of droplets moving in turbulent flows. The obtained results have been compared with the standard HDNS, i.e. without lubrication forces, and simulations in which the effects of AI were entirely neglected. The performed numerical experiments led to several original findings and conclusions. First, the importance of considering lubrication effects in droplet–droplet AI has been quantified. Second, it has been proved that a continuum representation of lubrication force is accurate enough for modeling dynamics of medium-sized cloud droplets. Third, the rigid particle assumption for water droplets in air is sufficiently precise, and there is no need to employ a fluid drop model for collision statistics. The performed simulations cover a fairly wide range of droplet mass loadings, so that the effect of liquid water content can also be assessed. Moreover, the outcomes from the simulations allow evaluating the impact of gravity on the droplet collision rate and other statistical parameters.

An alternative numerical method to account for AI relies on incorporating a two-way momentum coupling into the governing equations of fluid dynamics. With such a treatment, there is a mutual interaction between the fluid and particles. Consequently, not only does the air flow affect the droplets (via LPT), but also the motion of the droplets modulates the flow by a corresponding source term in momentum (Navier–Stokes) equations. The results from the simulations were validated against analogous simulations performed under one-way momentum coupling. When increasing the particle concentration (mass loading), a more uniform spatial distribution (lower RDF) has been observed along with a slight enhancement in the average relative velocity between droplets (higher RRV). In addition, the simulations have been performed on grids of different resolutions, corresponding to different domain sizes. The aim is to address the influence of the range of turbulent scales, identified by the Taylor-microscale Reynolds number, on the dispersed phase. A particular issue raised here is a prohibitively expensive computational cost for simulations with a large mass loading. This necessitates using a parametrization known as the super-droplet (particle parcel) approach, which significantly lowers the numerical complexity but reduces accuracy.

The results and discussions presented in this dissertation provide a quantified and comprehensive analysis of the influence of AI on the kinematics and dynamics of droplets interacting in turbulent air. This is a step forward in understanding the cloud microphysics, leading to the development of more accurate parametrizations for NWP models.

Keywords: cloud droplets, turbulence, DNS, aerodynamic interaction, lubrication force, collision statistics, two-way momentum coupling, cloud microphysics, environmental engineering, high-performance computing