Langevin Dynamics simulations of transport and aggregation of soot particles in turbulent flows

Abstract

Soot aggregates are emitted from many combustion processes as a result of incomplete combustion of a hydrocarbon. The hydrocarbon molecules nucleate through a complex series of chemical reactions and grow via surface addition mechanisms, e.g. surface reactions and condensation. The newly formed particles then mostly carried out in turbulent conditions, such that the particles adhere to each other when they collide due to their relative velocities induced by spatial velocity variations in the fluid flow and Brownian motion. Soot aggregates are found to be of very different sizes and shapes and their irregularity has a significant impact on their usually adverse final quality and environmental effects. Thus, an understanding of the aggregation process (i.e. particle motion, dependency of particle collisions, dependency of aggregates' structure and dynamics) on turbulent characteristics, such as turbulent kinetic energy, dissipation rate and fluctuation) is of primary importance. In this study, Langevin dynamics (LD) are used to track particle trajectories and collisions in turbulent flows with different flow and particle conditions that can be characterized by the Knudsen and Peclet numbers.