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Dynamics of nanoparticle aggregation and aggregate growth in turbulent flows

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The synthesis of nanoparticles in turbulent flames represents a cost-effective method for producing functional materials on a large scale. Depending on their size, surface area and morphology, these nanoparticles can exhibit remarkable properties that make them valuable commodities for a wide range of applications. Although flame synthesis is used routinely today, many underlying particle processes, including the formation of nanoparticle aggregates, are still not well understood. Consequently, current modelling strategies are often subject to significant uncertainties and only provide limited accuracy.

In the present study, we investigate the aggregation of nanoparticles in homogeneous isotropic turbulence by means of detailed numerical simulations. In particular, the trajectories of individual particles are directly resolved which allows for a direct, model-free treatment of collision events between aggregates. Further, particle dynamics are governed by the Langevin equation and incorporate the coupled effects of Brownian diffusion and turbulent shear. In addition, we retain the non-spherical, fractal-like structure of nanoparticle aggregates by keeping track of the primary particles within the aggregate.

The detailed, but costly, particle simulations are complemented by numerical solutions of the aggregation population balance equation. Within this statistical formulation, the temporal evolution of the aggregate size distribution is followed, however, a suitable expression for the coagulation rate coefficient is required. Our results indicate that standard models for the coagulation rate coefficient lead to considerable differences compared to the detailed simulation. In contrast, much better agreement is obtained when utilising an extended version of our recently developed coagulation rate model [1].

References

[1] Karsch, M. & Kronenburg, A. ”The collision kernel of nanoparticles in homogeneous isotropic turbulence: Direct simulations and modelling”. *Journal of Aerosol Science*. 2025; 186:106552.