Numerical simulations of dispersion and mass transfer in droplet-laden turbulent flows

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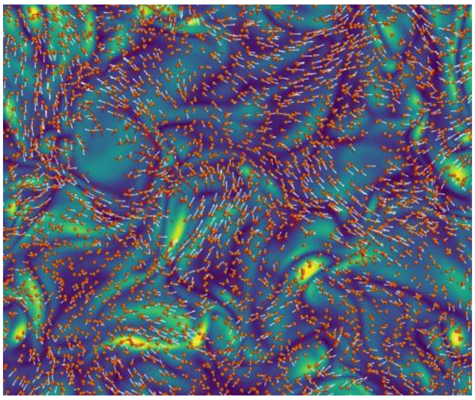

Vorticity field of the flow and particle preferential accumulation due to drag force and interia [4].

The understanding of physics and the prediction of heat or mass transfers in droplet-laden turbulent flows are crucial in a wide variety of engineering or environemental problems such as droplet growth in clouds, evaporation of turbulent sprays in combustion chambers or droplets containing a viral load, absorption of CO_2 or contaminated aerosols by spraying, liquid-liquid extraction for nuclear fuel reprocessing.... All these process engineering issues, which need to become more efficient, cleaner and safer, are sharing the complexity of coupling three physico-chemical phenomena: the multiscale and unsteady nature of turbulence, the heterogeneous dispersion of droplets (reliable force modeling), and the transfer of mass or heat between phases (interfacial flow modeling and phase change). In recent years, these three aspects have led to significant advances in the scientific community, and specifically in our team [1-3].

The objective of the PhD is to simulate turbulent flows by Direct Numerical Simulation (DNS) of the Navier-Stokes equations to spatially resolve all turbulent scales, in particular those controlling the transport of a passive scalar (Batchelor scale). The DNS solver will be coupled to the Lagrangian tracking of droplet trajectories. This approach has already been used in several PhD theses; recently A. Boutsikakis analyzed the effect of electrostatic forces on particle dispersion [4]. In the present PhD Thesis, we will take into account the latest developments of force modelling in the Lagrangian tracking of droplets, including the effects of lift and history forces (special case of drops [1-2]). Finally, to model interfacial transfer, we now have reliable closure laws for a wide range of Reynolds and Péclet values for liquid-liquid and gas-liquid systems [3].

With this simulation code, we will scrutinize three practical configurations with increasing complexity:

- CO_2 capture (or aerosols) by a cloud of droplets in free fall in a turbulent flow. Here, the gas-liquid transfer that drives the flow of absorbed material is depending on the preferential accumulation of droplets in specifics zones of the flow that are more or less loaded with passive scalar.
- The liquid-liquid transfer experienced by dispersed droplets in chemical engineering units during solvent extraction (possibly reactive extraction, internal droplet reaction to accelerate physical transfer).

- Droplet growth in a turbulent flow. Droplet growth leading to a heterogeneous size distribution occurs through droplet growth due to the humidity present in the carrier gas, and coalescence (drops of different sizes collide as they settle). This problem of micro-physics in clouds is still very poorly modelled by macroscopic approaches.

The numerical results will be compared with theories or experimental results (collab. Y. Hardalupas, Imperial College) and will improve the reliability of macroscopic modelling (Wunsch TI, 2009) of these complex phenomena, key elements in the design of more efficient and less polluting processes, or in the prediction of natural phenomena.

Candidates should have a strong education backgournd on fluid mechanics and multiphase flows, and an interrest for high performance numerical simulations (HPC).

References

[1] Shi P, Climent E and Legendre D (2024) Lift force on a spherical droplet in a viscous linear shear flow. Journal of Fluid Mechanics 1000, A88. https://doi.org/10.1017/jfm.2024.1072

[2] Godé H, Charton S, Climent E and Legendre D (2023) Basset-Boussinesq history force acting on a drop in an oscillatory flow. Physical Review Fluids 8(7), 73605. https://doi.org/10.1103/PhysRevFluids.8.073605

[3] Godé H, Climent E, Legendre D and Charton S (2024) Conjugate mass transfer from a spherical moving droplet: Direct numerical simulations of enhancement by a chemical reaction. Chemical Engineering Journal 489, 151073. https://doi.org/10.1016/j.cej.2024.151073

[4] Boutsikakis A, Fede P and Simonin O (2022) Effect of electrostatic forces on the dispersion of like-charged solid particles transported by homogeneous isotropic turbulence. Journal of Fluid Mechanics 938, A33. https://doi.org/10.1017/jfm.2022.189