Summary for ERCOFTAC “da Vinci” competition 2023

General information

Title of the work: Dynamics of bubbles across scales
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Keywords: Bubbly flows, DNS, multiphase, multiscale, lift force, scalar mixing

Popular science summary

Bubbly flows are important in many industrial and natural processes, such as chemical reactors, heat exchangers, and atmosphere-ocean exchanges. It is essential to accurately predict the bubbly flow dynamics to understand and design such systems. Numerical predictions of bubbly flows are very challenging, mainly because of their multiscale nature where processes at bubble (micro/millimeter) scales potentially interact with those at industrial scales (meters). The present research concerns numerical investigations of bubbly flow phenomena across a wide range of spatial and temporal scales. The aim is to increase our understanding of relevant bubbly flow phenomena and to facilitate improved predictions of bubbly flows at all relevant scales. First, we focus on the evolution of micrometer-sized vapor bubbles by formulating a multiphase Direct Numerical Simulation (DNS) framework and a computationally inexpensive 1D framework, which both involve phase change and thermal effects. These frameworks are used to study laser-induced thermocavitation bubbles, which are part of a promising technology to achieve good control of the properties of the formed crystals in the crystallization process. Our findings identify plausible mechanisms that induce crystallization and give guidelines for selecting suitable system parameters to control the crystallization process. We continue to larger scales by focusing on the dynamics of individual rising bubbles. An efficient multiscale methodology is developed that first predicts the liquid-phase fluctuations experienced by a bubble rising in a turbulent flow field in an Eulerian-Lagrangian framework. The dynamics and deformation of the bubble due to the liquid-phase fluctuations are then resolved using a DNS framework with a Moving Reference Frame (MRF) technique. This methodology is useful for studying numerous small-scale processes where bubbles are smaller than the turbulent length scales and can be used for bubbles, droplets, or particles in both laminar and turbulent flows. We use the developed DNS framework with the MRF to study the lift force acting on deformable bubbles in steady shear flows. We formulate a theoretical framework based on vorticity dynamics and support it with simulations to provide a comprehensive explanation for all identified mechanisms behind the lift force. The findings also elucidate the influence of the shear rate on the lift force. Finally, we numerically study the dynamics and mixing properties of passive scalars in turbulent bubbly flows, such as heat or chemical species in heat exchangers or bubble column reactors, at large spatial scales (size of the entire simulation). We identify four interacting mixing mechanisms and extract scalar statistics that show how bubbly flows provide an efficient means of scalar mixing and transport. We also find a significant influence of the bubble-induced turbulence and the governing parameters on the scalar dynamics and mixing properties. In summary, the present research increases our understanding of many important bubbly flow processes and provides general numerical frameworks for studying bubbly flows across scales.

Scientific summary

The main objective of the research is to increase our general understanding of relevant physical phenomena in bubbly flows and to improve numerical predictions over a wide range of spatiotemporal scales. An illustration of such phenomena, length scales, and the associated publications are shown in Figure 1, left panel. In all the papers, the Volume Of Fluid (VOF) multiphase DNS technique is used and is henceforth referred to as DNS. At the smallest considered scales, we study the evolution of micrometer-sized vapor bubbles. We focus on laser-induced thermocavitation, which is currently studied as a promising tool for controlling the crystallization process and exemplifies the challenges and complexities encountered in both boiling and cavitation processes. Here, we identified a need for a better understanding of the fluid conditions in and around the bubble to explain the mechanism behind the experimentally observed crystallization. We develop two numerical frameworks, a DNS framework with interfacial phase change modeling [1] and a corresponding 1D numerical framework that resolves the relevant fluid conditions. We use the numerical frameworks to study the fast and complex dynamics of a laser-induced thermocavitation bubble with growth rates governed by a rapid phase change and thermal effects at the bubble interface. Figure 1, center panel, illustrates the DNS results and shows that the rapid solvent evaporation during the early bubble growth phase produces a peak of solution supersaturation at the bubble interface that is impossible to obtain using conventional crystallization techniques under normal conditions [2]. Since crystals have a higher probability of nucleating at increased supersaturation levels, our results indicate that the predicted peak due to rapid solvent evaporation may be the mechanism behind the observed crystallization. We also perform an extensive parameter investigation of the effects of the laser pulse energy, the spatial distribution of that energy, the solute diffusivity, and the solute solubility on the maximum supersaturation level obtained during the bubble evolution process. The findings show that high supersaturation peaks are only obtained under specific ranges of the studied parameters. Guidelines are provided to identify suitable sets of parameters that produce conditions favorable for crystallization.

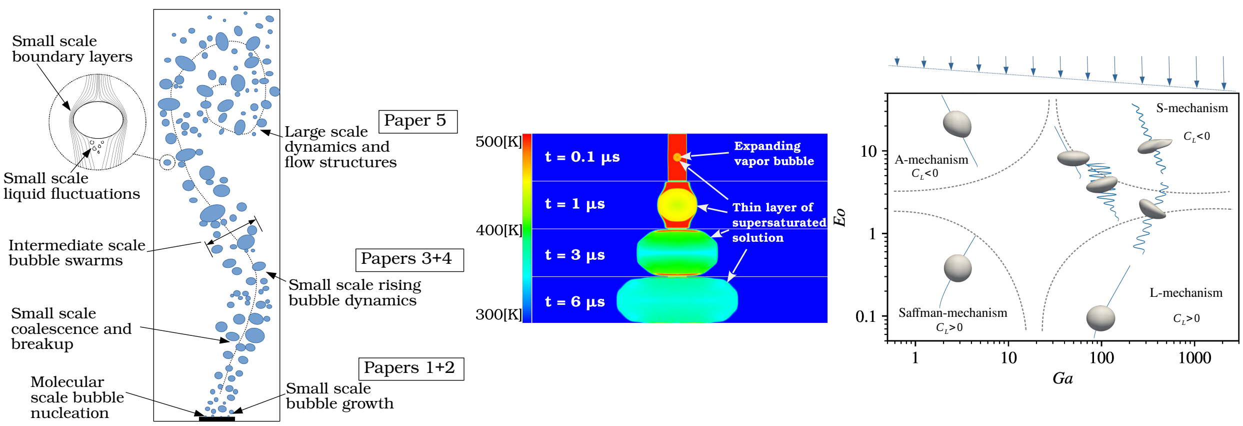

Figure 1: Left panel: illustration of bubbly flow processes occurring at various length scales during saturated nucleate pool boiling and indication of the scales and processes addressed in the respective papers. Center panel: temperature field around a growing laser-induced vapor bubble after a cylindrical laser pulse superheats the solution. Right panel: (Ga, Eo)-phase plot illustrating the different behaviors of the lift force with the governing parameters and the regions of the phase space governed by the different lift force mechanisms.

We then shift the focus to the dynamics of individual rising bubbles, where the dynamics may develop over large spatiotemporal scales. To expedite simulations, we develop a multiscale methodology that predicts the motion of a sub-Kolmogorov bubble in fully resolved turbulence using an Eulerian-Lagrangian solver. The turbulent fluctuations experienced by the bubble are imposed on a DNS solver with a Moving Reference Frame (MRF) technique that follows the rising bubble. The DNS solver thus resolves the detailed small-scale bubble dynamics in response to the realistic turbulent fluctuations. With this approach, the cost of DNS is significantly reduced, and the setup of the simulations is simplified by eliminating the need for a priori estimations of sufficient domain sizes to capture the bubble dynamics. The methodology can be used to study many small-scale processes for bubbles, drops, or solid particles in turbulent and laminar flows. Such studies can elucidate the effects of the liquid flow on the small-scale dynamics and facilitate improved models.
We use the DNS and MRF techniques to extensively study the lift force acting on a deformable and freely moving bubble rising in linear shear flows [4]. The lift force governs the spatial distribution of bubbles in relevant bubbly flow systems such as bubbly pipe flows and affects the flow stability in bubble columns. A thorough understanding and accurate models for the lift force are thus crucial to design efficient bubbly flow applications. The lift force is a complex function of the governing parameters and may even change sign at increasing bubble deformations. Consequently, the lift force coefficient C_L varies highly non-linearly with the governing parameters. This complex behavior is due to the interaction of four identified lift force mechanisms, some of which we only recently have begun to understand. The main objective of our study is to provide a general description of the four mechanisms and qualitatively explain how the mechanisms cause the complex lift force behavior in the relevant phase-space of the governing parameters (the Galilei Ga and Eötvös Eo-numbers). We also aim to elucidate the effect of the shear rate on the lift force induced by the different mechanisms. To explain the lift force mechanisms, we provide a theoretical framework that relates the lift force acting on the bubble to moments of bubble-induced liquid vorticity. The theoretical considerations are then supported by the DNS. The findings provide a novel and comprehensive explanation for all mechanisms in terms of their characteristic bubble-induced vorticity fields. Figure 1, right panel, shows qualitatively the regions of the phase-space dominated by the different mechanisms and explains the complex lift force behavior within the phase space. The numerical results also show that the shear rate significantly

influences the lift force coefficient in highly viscous flows or at significant bubble deformations and should thus be accounted for when formulating closures for the lift force.
Lastly, we explore the dynamics and statistics of passive scalars, such as heat or chemical species, in bubble-induced turbulence across large scales (systems with $O(10-100)$ bubbles in periodic domains) [5]. The main objectives are to determine how the bubble-induced turbulence modifies the scalar spectra and study the scalar spectra energy budget to elucidate the mechanisms behind the observed scalar spectra behavior. We also assess the influence of the governing parameters on the scalar spectra and the effective scalar diffusivity of the bubble suspension. These objectives are essential when developing accurate models of scalar dynamics in industrial-scale systems. We develop a DNS framework with a repulsive force model to prevent bubble coalescence and preserve a monodisperse bubble size distribution over long simulation times. A snapshot of the scalar field from DNS is shown in Figure 2, left panel. From the simulations, we extract statistically steady quantities of the velocity and scalar fields. Figure 2, right panel, shows the scalar fluctuation spectra and demonstrates that the bubble-induced turbulence induces a transition of the scalar spectra from the $k^{-5/3}$ scaling (observed in single phase isotropic turbulence) to the k^{-3} scaling, with the wavenumber k, characteristic for the velocity spectrum of bubble-induced turbulence. The transition length scale for the former spectra is comparable to or smaller than the bubble diameter and decreases with the molecular diffusivity of the scalar in the liquid (increasing liquid Schmidt number Sc_l). By using DNS, we resolve all scales down to the diffusive dissipation scales. This allows us to analyze the scalar transfer term in the scalar budget equation and show that this term scales as approximately k^{-1} at the scales below the bubble diameter and induces the k^{-3} scaling of the scalar spectra. We have also found that the gas scalar diffusivity may significantly influence the scalar fluctuations of the suspension. This effect influences the convective scalar diffusivity for which we propose scalings based on a priori known governing parameters. The findings increase our understanding of scalar transport in turbulent bubbly flows and aid the development of improved models to predict the scalar dynamics in large-scale industrial systems such as heat exchangers and bubble column reactors.

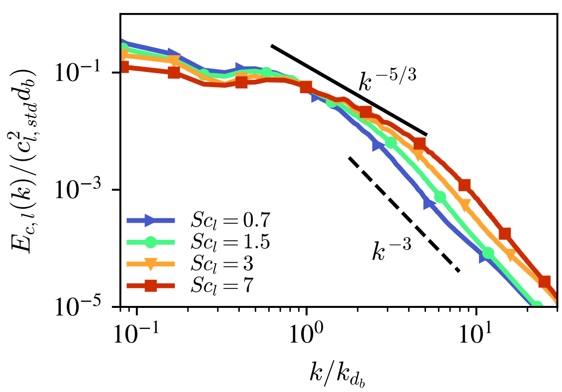

Figure 2: Left panel: Contours of the scalar field in a turbulent bubbly flow with a gas volume fraction $= 5.2\%$ and a mean scalar gradient in the vertical direction. Right panel: Corresponding scalar fluctuation spectra at various liquid Schmidt-numbers Sc_l.

List of main pubblications

1. N. Hidman, G. Sardina, D. Maggiolo, H. Ström, and S. Sasic. Laser-induced vapour bubble as a means for crystal nucleation in supersaturated solutions - Formulation of a numerical framework. *Experimental and Computational Multiphase Flow*, 2019, 1.4, 242-254.

2. N. Hidman, G. Sardina, D. Maggiolo, H. Ström, and S. Sasic. Numerical Frameworks for Laser-Induced Cavitation: Is Interface Supersaturation a Plausible Primary Nucleation Mechanism? *Crystal Growth & Design*, 2020, 20.11, 7276-7290.

3. N. Hidman, H. Ström, S. Sasic, and G. Sardina. A multiscale methodology for small-scale bubble dynamics in turbulence. *International Journal of Multiphase Flow*, 2022, 150, 103976.

4. N. Hidman, H. Ström, S. Sasic, and G. Sardina. The lift force on deformable and freely moving bubbles in linear shear flows. *Journal of Fluid Mechanics*, 2022, 952, A34.

5. N. Hidman, H. Ström, S. Sasic, and G. Sardina. Assessing passive scalar dynamics in bubble-induced turbulence using direct numerical simulations. *Journal of Fluid Mechanics*, 2023, 962, A32.