PhD Thesis from October 2024, <u>or</u> 2-year **Postdoctorate**

Numerical simulation of nucleate boiling: from bubbles towards the macroscopic scale

Context

Storage and transport of liquid energy vectors (hydrogen in particular, but also methane, oxygen, …) are critical aspects of both energy transition and space exploration. The liquid state of these fluids is found at very low (cryogenic) temperatures, so that they boil due to the heat flux from the environment. Despite their deep environmental and economic implications, several aspects of the behavior of cryogenic multiphase fluids in tanks are not well understood, in particular the effects of phase change (boiling and condensation) and wetting properties on the dynamics, and its feedback on mass and energy transfer between phases, ultimately producing mass losses in the tanks. This is a key point for mastering ground hydrogen storage and delivery [Moradi 2019], rocket launches, long-distance space missions including in space depots [Hadler 2021], but also LNG transport in tankers: in general, cryogenic tanks from 0g to multiple-g gravity.

In presence of a heat flux coming from the container walls, bubbles nucleate at the walls (this phenomenon is called nucleate boiling) and absorb heat, that is then transported in the bulk liquid when bubbles detach. This is a complex problem in fluid mechanics (the overall evolution of the system depends on the position of the liquid-vapor interface that is not known a priori, and that exhibits in general a complex dynamics), and on the top of that it is also a multi-physics (fluid mechanics, thermodynamics) and multi-scale problem (the solid-liquid-vapor contact line dynamics depends on molecular-scale properties; bubbles are typically in the millimeter range; the flow structures go from below the bubble size to the system size) that is still not well understood.

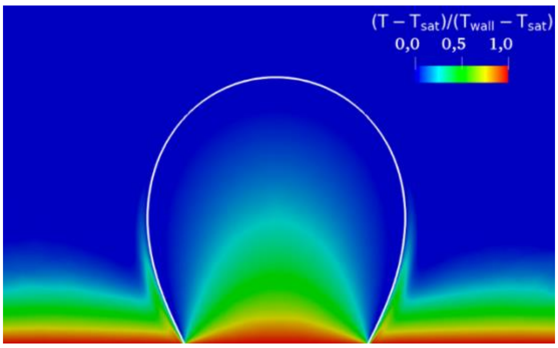

Figure 1 : Simulation of a water vapor bubble during boiling at ambient pressure, fluid interface and temprature field (from [Pertant 2022]).

The present project addresses the multi-scale issue, taking accurately into account the fluid mechanics and the multi-physics couplings. It takes advantage of the numerical solver for boiling flows at the bubble scale, developed during the last years by the MoST team [Sahut 2021, Pertant 2022] within the high-performance computing platform YALES2 (a general-purpose collaborative CFD code co-developed by several research laboratories and industrial partners in France and abroad, https://www.coria-cfd.fr/index.php/YALES2). It aims to achieve numerical simulations that go beyond the scale of one or few bubbles, by developing subgrid-scale models that allow to consider bigger systems, typically a large amount of bubbles in hydrodynamic and thermal interaction. From a fundamental point of view, this will help to shade light on the physical mechanisms that contribute to heat transport from bubbles to the system scale. Overall, this project will contribute to the long-term energy stakes in energy storage and transport.

The project is part of the MacroBoil project (Macroscopic numerical models for Boiling and condensation, funded by the French Agence Nationale de la Recherche from 2024 to 2028), in partnership with CORIA and IMFT laboratories, and ISAE-SUPAERO, and in collaboration with ArianeGroup.

Project organization

The project is structured as follows:

- First, the existing numerical code will be used to simulate nucleate boiling on highly refined meshes, allowing to capture the thin thermal boundary layer around the bubbles and then compute the rate of vapor production. This will allow to create a reference dataset to be compared with results obtained by partners IMFT and ISAE-SUPAERO [Huber 2017, Urbano 2018] that use a different numerical approach. The dilatability of the vapor phase may also be taken into account at this stage.
- Then, in collaboration with the other MacroBoil partners and in particular with CORIA [Atmani 2021, Pecquery 2022], numerical models of the rate of vapor production will be developed and used to simulate the growth of single or few bubbles on coarser mesh, and validated.
- Finally, simulations containing many bubbles will be performed and analyzed, allowing for a physical analysis of heat transfer taking into account the collective effects.

Funding and material conditions

The PhD/postdoctorate funding is granted. The recruited person will join the MoST team at LEGI, and will benefit of a stimulating and dynamic environment. Access to local and national computing facilities will be provided, as well as technical support for simulations. He or she will have opportunities to present the obtained results to national and international conferences, as well as to publish the results in peer-reviewed journals.

Location

Laboratory LEGI, MoST team, University Grenoble Alpes, Grenoble, France.

Application

The candidate is expected to have a Master's degree (for the PhD) or PhD (for the postdoctorate) with knowledge in fluid mechanics and a marked taste for physical modelling, numerical methods, code development in a high-performance computing (HPC) environment.

To apply, candidates are required to send their curriculum vitae, motivation letter to the contacts listed below. For the PhD applications, please also include full academic grade transcripts. For the postdoctoral application, a one-page description of the PhD work is also expected. Applications from non-European candidates must undergo a security screening that will impose a 3-month delay in the recruitment process.

Contacts

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References

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