



Multiphase and thermodynamics numerical modelling of LH2 phase change

Research engineer position

Duration : 18 month

Salary : 2500€ gross

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In the context of decarbonation of industry due to climate change and energy transition, it is crucial to reinforce and develop efficient low-carbon engineering systems for the energy and transport sectors. A large quantity of applications involves compressible multiphase flows characterized by complex multi-physic and multi-scale interactions, that are fully challenging to model. The ANR project COMPET (COMPRESSible multiphase flow modelling for Energy and Transport applications) aims at bringing a contribution to the modelling and the physical analyses of such multiphase problems.

In particular, hydrogen is currently being deployed to replace fossil fuels in various sectors. However, its very low volumetric energy density means that it must be used in liquid phase under **cryogenic conditions** (LH2 around 20 K). It needs to adapt the power supply chain, using for example compact pump operating at high speed, in which vaporization occurs. Despite the efforts made in this field, the numerical simulation of cavitating flows in LH2 still presents significant scientific challenges in terms of thermodynamic description (equation of state - EOS), modelling of non-isothermal phase transition (coupled mass and heat transfer between phases), the presence of intense pressure waves and the complex interaction with turbulence.

In this context, the post-doc aims to contribute to the modelling of compressible multiphase problems related to the development of hydrogen-powered technologies for low carbon applications. The work focuses on the SCB diffuse interface compressible code, which contains a hierarchy of multiphase models: 4-equation, 5-equation and multicomponent models, integrated in a fully parallel environment [1].

We propose to jointly address the following challenges:

- **Test different EOS for liquid hydrogen**

LH2 in cryogenic conditions shows complex thermodynamics behaviour. It will be necessary to introduce temperature-dependence for the fluid properties: saturation pressure, viscosities, heat capacities (for example [2]). We will explore different EOS of increasing complexity to represent the fluid: Noble-Abel Stiffened Gas [3], Murnaghan and variants. In addition, we will test the open-source library CoolProp [4] which proposes tables at thermodynamic equilibrium for LH2 in cryogenic conditions.

- **Develop well-posed models for phase transition**

The plan is to compare and develop physical models, in terms of mass transfer coupled with heat transfer. The HRM, based on a four-equation formulation, will be investigated by varying the relaxation time. It will be compared to the 5-equation formulation in which the heat transfer term appearing in the void ratio equation will be closed. A first validation will be carried out on canonical configurations with low Reynolds numbers for which data are available in the literature : i) 2D cylinder case in laminar regime involving vortex-cavitation and thermal effects [5], ii) LH2 cases of NASA (2D hydrofoil and ogive) for which wall temperature and pressure distributions are available [6].

- **Perform high-fidelity simulations of canonical flows**

Different 3D cases at moderate Reynolds number will be computed using an implicit sub-grid strategy (ILES) [7] in order to better understand the physical phenomena, the complex self-sustained and instability mechanisms, for a better design of these systems.

- **Promote the results** by writing scientific articles, preparing presentations, and participating in project meetings.

Profile

With a Ph.D. degree, you have solid scientific expertise in computational fluid dynamics and two-phase modelling, as well as in computer science (programming, processing large volumes of data, high-performance computing). Knowledge of numerical methods for compressible flows would be a plus.

The candidate must demonstrate scientific independence and the ability to work independently while collaborating with a multidisciplinary project team.

References

- [1] Goncalves & Parnaudeau, "Comparison of multiphase models for computing shock-induced bubble collapse", *Int. J. Num. Meth. Heat Fluid Flow*, Vol.22, 2020.
- [2] Li, Yu, and Kadam, "An improved cavitation model with thermodynamic effect and multiple cavitation regimes", *Int. J. Heat & Mass Transfer*, 205, 123854, 2023.
- [3] Le Métayer and Saurel, "The Noble-Abel Stiffened-Gas equation of state", *Phys. Fluids*, 28, 046102, 2016.
- [4] Bell et al., "CoolProp: An open-source reference-quality thermophysical property library", In: *ASME ORC 2nd Int. Seminar on ORC Power Systems*, Rotterdam, Netherlands, 2013.
- [5] Dinh Le, Truong and Iga, "Thermodynamic cavitation suppression on the laminar vortex flow over a circular cylinder in water", *Int. J. Heat & Mass Transfer*, 211, 124210, 2023.
- [6] Hord, "Cavitation in liquid cryogenics," *NASA report CR-2156*, 1973.
- [7] Tenaud, Parnaudeau and Goncalves, "Toward the numerical study of the vortex cavitation behind a cylinder at Reynolds number of 3900", *Int. Conf. on CFD*, Milan, July 2026.