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Calibration and verification of CFD-VOF models for the analysis of pressurization scenarios in LH_2 tanks

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Abstract. Due to its high power density, the aviation sector is pushing towards its electrification by designing new propulsion systems based on cryogenic liquid hydrogen (LH_2). From an engineering point of view, the efficient design of tanks constitutes one of the main challenges. They must guarantee efficient isolation of the hydrogen to avoid its evaporation and, at the same time, ensure reasonable weight and dimensions. Using numerical simulations is fundamental for studying heat transfer between the external environment and the liquid fuel. This work focuses on the simulation of multiphase liquid-gas flow to analyze the tank pressurization as a function of different external heat fluxes. A commercial CFD software is used to perform simulations. VOF simulations with the Lee mass transfer model are employed, and some critical numerical parameters are analyzed to provide information on the optimal values.

1. Introduction

According to recent research trends, electrification in different transportation fields will pass through hydrogen-powered propulsion. To guarantee the necessary quantity of fuel within limited storage spaces, the hydrogen must be stored in liquefied form and isolated from the external environment. The H2ELIOS project will develop a lightweight, innovative, and efficient LH_2 aircraft storage prototype, ready to be integrated into the aircraft architecture for flight demonstrations at later stages. Hydrogen tanks would be subjected to highly variable conditions in terms of pressure and temperature, as well as sloshing effects, triggering drastic evaporation and condensation processes. High-fidelity simulations constitute a fundamental tool for studying basic concepts in this field.

Phase change processes are represented in CFD through two main types of models: two fluid models and interface-capturing models. In two-fluid models, vapor-liquid two-phase flow systems are represented on an Eulerian-Eulerian framework, thus employing the same mesh for discretizing governing equations. Both phases are described using mass, momentum, and energy conservation equations and are considered interpenetrable. The mass, momentum, and heat exchange between two phases are detailed by introducing closure relations that model the interaction between phases. Momentum exchange closures include drag and lift forces, turbulent dispersion, wall lubrication, and virtual mass. Additional semi-empirical terms must be modeled to consider the effect on momentum and energy equations of bubble nucleation frequency and size, interfacial and turbulent heat transfer, and wall boiling models. Two-fluid models have reached popularity mainly thanks to studies related to nuclear reactor safety, in particular, to accurately predict the appearance of critical heat fluxes on pipes and fuel rod bundles. Consolidated models are already available in the most common simulation packages (Fluent/CFX, Star-CCM, or OpenFOAM) to analyze boiling flow phenomena, especially those related to thermo-nuclear problems. Nonetheless, this class of models does not appear to be adequate for the study of evaporation and condensation phenomena necessary to represent the boil-off of dormancy processes, especially in cases where, as in LH_2 tanks, considerable fluid compression is expected.

The models corresponding to the second leading group (interface-capturing methods) are characterized by a scalar function that embeds the moving interface on a fixed grid. The interface-capturing approaches employ only one set of equations to describe the different phases, while the interface is captured using scalar functions. The two main interface-capturing options are the Volume-of-Fluid (VOF) and Level-Set methods. Most works dealing with LH_2 evaporation processes are based on VOF or Level-Set methods developed within commercial software. A significant unknown is the approach employed for calculating the interface mass transfer. The most used model, available by default in commercial software, is the Lee equation, used in several works such as Li et al. [1] and Jiang et al. [2] for LH_2 studies. In Lee, the mass transfer rate is proportional to the difference between the local and saturation temperatures, driving the phase change process. However, the mass flow is proportional to the accommodation coefficient β, defined empirically, that needs to be fine-tuned to match experimental data. However, other options have been developed as user-defined functions (UDFs); for example, the Schrage model is employed by Kartuzova et al. [3] and Stewart et al. [4], while the Collier and Thome model is adopted by Shihao et al. [5].

The current work focuses on calibrating VOF schemes when applied to pressurization events. Particular attention is given to the role of pressure and accommodation coefficient. Hence, the model is verified compared to the experimental reference from Aydelott [6].

2. Numerical model

Preliminary tests were performed using a compressible phase change model based on two-fluid formulations available in the open-source software OpenFOAM. Those tests have helped to assess the low suitability of two-fluid models in simulating boil-off hydrogen phenomena, mainly due to the excessive artificial diffusion at the interface.

For this reason, the choice of employed software finally went to Ansys Fluent Version 22. A 2D axisymmetric domain reported in figure 1(a) was used to reproduce the spherical domain employed in the experimental work from Aydelott [6] and represents a sphere with diameter $d = 0.22$ m. The VOF model with the modified High-Resolution Interface Capturing (HRIC) convective scheme is selected to represent the two-phase flow interface. No turbulent modelization is employed in the momentum equations at this stage. A Pressure-Implicit with Splitting of Operators (PISO) scheme is used for the pressure-velocity coupling with explicit time advancement and fixed time-step. Quadratic Upstream Interpolation for Convective Kinematics (QUICK) convective schemes are employed to solve Momentum and Energy, while the PREssure STaggering Option (PRESTO!) algorithm is employed for pressure resolution. The gas is considered ideal, while the Boussinesq model is employed to evaluate buoyancy effects in the fluid. Variations of properties with temperature and pressure are set using UDFs.

3. Validation tests

As commented the performed numerical tests reproduce the experimental set-up from Aydelott [6]. The mesh accounts for 7480 nodes, and the final size was chosen after a mesh convergence analysis. The mesh is densified around the wall boundary to allow a more precise calculation of wall heat fluxes and in the interface zone to allow a sharper representation of the free-surface and interfacial mass transfer phenomena. All the cases analyzed have a similar initial filling percentage, hence, the same mesh is employed for all the cases.

Initial tests helped select proper numerical parameters as the time-step, Δt, and the accommodation parameter of the Lee model, β. The chosen test for preliminary analysis was Test 3 from Aydelott [6], characterized by q = 144 W/m^2 in the dry zone and q = 253 W/m^2 in the wet one. Pressurization results are reported in figure 1(c) and figure 1(b). Regarding Δt, a sufficient convergence was reached for $\Delta t = 0.001s$. The β coefficient, defined as a time-relaxation parameter in Fluent manuals and literature, was found to affect only the initial transient evolution, while the pressure rise rate after the initial transient was found to be very close between the different cases analyzed, as depicted in figure 1(b). In particular, we can see how $\beta = 0.1$ and $\beta = 0.01$ cases directly lead to flow pressurization, with a similar slope of the rise rate. When using $\beta = 1.0$, the flow experiences an initial depressurization, probably due to the condensation of part of the gas volume; however, the process is soon reverted as the gas receives energy and starts pressurizing at a rate very similar to the past two cases. The value chosen for the following simulation was the default, $\beta = 0.1$.

Finally, three simulations were carried out, reproducing different energy input levels within the system, and using the set of numerical and physical parameters selected previously. The cases investigated are classified with the original numbering shown in [6]. In particular, Tests 1, 3, and 6 are analyzed, mainly varying in terms of heat fluxes set as boundary conditions at the external wall. Different heat fluxes are set for the wet (filled with liquid hydrogen) and dry (in contact with gas) zones, thus mimicking the conditions imposed by Aydelott [6] as truthfully as possible. The results in terms of pressure rise rate are reported in figure 1(d), however, the quantitative validation is done by comparing the rise rates reported in table I of [6]. The results are reported in table 1 showing how the pressure rise rate closely matches the experimental value in all the analyzed cases (with a slight over-prediction).

4. Conclusions

In this work, numerical tests were performed on a commercial platform aimed at measuring the degree of pressurization of cryogenic liquid hydrogen tanks subjected to different levels of heat flow. The numerical set-up mimics the experimental test proposed by Aydelott [6]. This paper reports the numerical parameters obtained in preliminary simulations, which allowed the model to be calibrated. Furthermore, sensitivity analyses towards certain fundamental parameters such as the accommodation coefficient, β, or the time-step are reported. Finally, hydrogen pressurization is validated under a wide range of boundary conditions regarding heat fluxes in the walls, closely matching the pressure rise rates obtained on the reference experimental work.

Table 1. Pressurization rate: comparison between numerical results and experimental reference [6].

	Q $[W/m^2]$ (wet/dry)	Exp. p rise rate $[Pa/s]$	Num. p rise rate $[Pa/s]$
Test 1	55/49	402	440
Test 3	253/144	1298	1382
Test 6	466/235	2218	2207

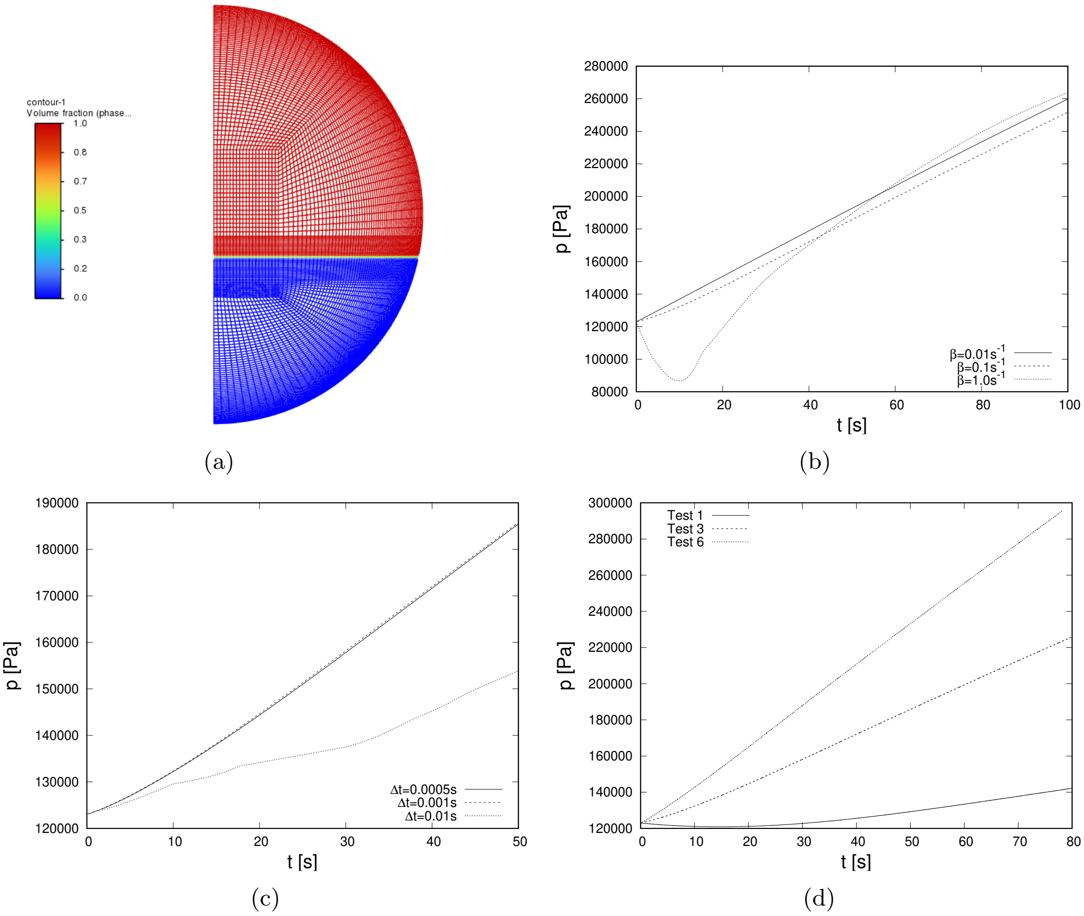

Figure 1. (a) Axisymmetrical domain employed to reproduce Aydelott [6] tests; (b) Parametric analysis of the accommodation coefficient, β (Test 3); (c) Parametric analysis on time-step (Test 3); (d) Pressurization of the tank under different heat fluxes (Tests 1,3 and 6).

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