

# Influence of buoyancy and wall heat transfer in CFD modelling of liquefied hydrogen storage tanks

Johan R. Espelund<sup>a,b,\*</sup>, Åsmund Ervik<sup>b</sup>, Svend Tollak Munkejord<sup>b</sup>, Magnus Aa. Gjennestad<sup>b</sup>, Luca Brandt<sup>c</sup>,  
Corinna Schulze-Netzer<sup>a</sup>

<sup>a</sup>Department of Energy and Process Engineering, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

<sup>b</sup>SINTEF Energy Research, P.O. Box 4761 Torgarden, NO-7465 Trondheim, Norway

<sup>c</sup>Department of Environment, Land and Infrastructure Engineering (DIATI), Politecnico di Torino, Turin, 10129, Italy

---

## Abstract

To employ liquefied hydrogen (LH<sub>2</sub>) for large-scale storage and transportation of low-carbon energy, boil-off prediction in cryogenic tanks is crucial. Boil-off is driven by heat ingress from the ambient, which also leads to pressurization and thermal stratification in the ullage. In this work, a sharp-interface model is implemented in OpenFOAM and used to predict pressurization, stratification and boil-off rates at three different fill levels of an LH<sub>2</sub> tank. A buoyancy source term is also implemented and added to existing RANS models. This source term is shown to completely suppress turbulence in the ullage. We have performed a series of simulations, predicting pressurization rates and thermal stratification. The results were compared to the K-Site experiments and for the first time, reasonable agreement was obtained across all fill levels. The boil-off rate showed qualitative agreement with the experimental estimates but was underpredicted in magnitude. The effects of heat-flux distribution, thermal contact resistance and variable wall thickness are also assessed, and their impact was found to be significant. This motivates the need for improved thermal boundary conditions, as well as possible coupling with resolved thermal models of the tank structure and insulation.

**Keywords:** CFD, cryogenic storage, tank pressurization, boil-off, liquefied hydrogen, turbulence

---

## 1. Introduction

With the green transition comes the need for large-scale energy storage due to the intermittency problem of renewable sources such as wind and solar. In this regard, hydrogen has emerged as a promising low-carbon energy carrier [1]. At ambient conditions, however, the density of hydrogen is very low, which is problematic in applications where volume is a constraint, such as in transport systems and space or aviation applications. In these applications liquefied hydrogen (LH<sub>2</sub>) is attractive, with a density almost 900 times higher than that at atmospheric conditions. The drawback of this approach is the low boiling temperature of hydrogen at around 20 K, which leads to high liquefaction costs; around one third of the energy content is spent on liquefying it, though some of it can be recovered during regasification. The low temperature also means that LH<sub>2</sub> is highly susceptible to heat ingress from the ambient, causing evaporation, which is often referred to as *boil-off*. Controlling boil-off is crucial due to the high energy cost of liquefaction, and achieving this requires improved understanding of the boil-off process [2].

In a context where experiments are scarce due to cost and safety constraints, modelling is key to understand-

ing the behaviour of LH<sub>2</sub> tanks. In general, methods for modelling LH<sub>2</sub> tanks (or cryogenic storage tanks) can be categorised into two classes: nodal models and computational fluid dynamics (CFD) models. Nodal simulations range from simple 0D models, where each region of interest (liquid, ullage, interface, walls, etc.) is represented by a single node [3], to 1D models that discretise the domain along the vertical direction and solve conservation equations for mass and energy [4]. The main advantage of nodal models over CFD models are their low computational cost, enabling the simulation of large-scale tanks over extended periods of time. A recent review of modelling of both storage and transfer of LH<sub>2</sub> is given by Claussner et al. [5].

A common feature of most nodal simulations is the use of empirical correlations to close the system of equations. Of particular importance are the heat-transfer coefficients on both sides of the liquid–vapour interface, which control the tank’s boil-off rate. There is no universally accepted correlation in the literature, and the appropriate value likely depends on tank geometry, fill level, and insulation heat ingress. As a result, different strategies are employed: some studies apply correlations for infinite horizontal surfaces [6], while others introduce a constant scaling factor calibrated against experimental data [7, 3]. Consequently, these models are typically limited to cases for which suitable experimental data are available for tuning the correlations.

---

\*Corresponding author

Email address: johan.espelund@sintef.no (Johan R. Espelund)

Some authors have combined the two strategies, modelling one of the phases with CFD while representing the other as using a nodal approach [8, 9, 10, 11].

Increasingly, LH<sub>2</sub> tanks have been simulated using two-phase CFD models, particularly in studies of thermal stratification and self-pressurization in closed tanks. Due to the higher computational costs, however, the tank size and simulation period tend to be limited compared with nodal simulations. A recent review of both CFD and experimental works on closed LH<sub>2</sub> tanks is given by Wang et al. [12]. In general, validation of CFD models has proved difficult because experimental data for LH<sub>2</sub> tanks are scarce, and the available instrumentation is often insufficient to fully specify the boundary and initial conditions required for the simulations. One of the most widely used experiments for validation is still the K-Site experiments performed by NASA in the 1990s [13, 14, 15], that have also been used for model validation by several authors [11, 16, 17, 18].

Due to the axisymmetric geometry and boundary conditions of cylindrical and spherical storage tanks, most CFD models of LH<sub>2</sub> storage tanks employ axisymmetry. When modelling both liquid and vapour phases, the Volume of Fluid (VoF) method is frequently employed with the Schrage phase change model [19]. As an alternative to VoF some authors have also utilised a *sharp-interface* approach [20, 21], where the vapour and liquid phases are treated as single-phase regions separated by a fixed interface. This approximation is well-suited for free-surface flows in which interface deformation can be neglected, such as in stationary storage applications. Compared to interface-capturing methods such as the Volume of Fluid (VoF) approach, the sharp-interface formulation substantially relaxes the spatial and temporal resolution requirements.

A recent study by Fernandes et al. [18] compared different phase-change models using VoF in axisymmetric CFD simulations of LH<sub>2</sub> pressurization and found a strong dependence of the results on the chosen phase-change model. The 49 % fill level from the K-Site experiments was used for validation. The Schrage model was found to match the experiments much closer than the other phase-change models, which significantly underpredicted pressurization after the first few hours. The Schrage phase-change model was compared with the equilibrium phase-change model in the sharp-interface simulations of Kassemi et al. [20]. In the equilibrium model, the interface is assumed to remain at the saturation temperature, and the two models were found to give nearly identical predictions.

An important aspect that has received continuous attention is on the role of turbulence. Cryogenic storage tanks are commonly found to be above the critical Rayleigh number for transition to turbulence, so turbulence modelling is employed [9, 22]. The CFD simulations by Rossetti et al. [22] of LN<sub>2</sub> tank experiments [23] found that the pressurization predictions were significantly improved by using the realizable  $k - \epsilon$  turbulence model over a laminar simulation. However, they also found that uncertainties in the specified heat flux to the tank were large enough

to cause discrepancies of the same magnitude. On the other hand, Kassemi et al. [24] found that *not* employing a turbulence model provided the best results when validating their model against the K-Site experiments, even though the Rayleigh number was above the critical value also in this case. Using the  $k - \omega$  Shear Stress Transport (SST) turbulence model [25], both pressurization and thermal stratification in the ullage was significantly underpredicted. Recently Kartuzova et al. [17] found that the Improved Delayed Detached-Eddy Simulation (IDDES) model gave improved results. The model predicted pressurization and thermal stratification with good results at low and medium fill levels, but both were underpredicted at the highest fill level. This was, however, also the case for the laminar simulation. Using a non-uniform heat flux on the tank wall improved the behaviour to some extent, but worsened the results at the lowest fill level.

Kartuzova and Kassemi [26] investigated the impact of conjugate heat transfer for the 49 % fill level and found that including tank wall conduction is crucial even in thin-walled tanks. They also found that accounting for variable wall thickness around weld lands and lid attachment improved the predicted pressurization rate. The importance of conjugate heat transfer was also demonstrated in simulations of LN<sub>2</sub> storage tanks by Rossetti et al. [22].

It is often challenging to evaluate the effect of modelling errors due to significant uncertainty in the boundary conditions. Consequently, the most suitable turbulence modelling approach remains unclear, and predicting stratification and pressurization over a range of fill levels using a consistent approach remains challenging.

In this work, a sharp-interface approach is used to model pressurization and stratification in the K-Site experiments, with the aim of increasing the understanding of turbulence effects and thermal boundary conditions. First, the influence of including a buoyancy production term in different RANS models is assessed and compared against DNS data [27]. The sharp-interface model is then applied to simulate pressurization and thermal stratification in the K-Site tank across all available fill levels. A 1D analysis of the experimental data also allows for comparison with the boil-off rate for the two highest fill levels. The influence of the buoyancy production term is then assessed, and the sensitivity to the heat-flux distribution, thermal contact resistance and variable wall thickness is investigated.

The rest of this paper is organised as follows. Section 2 describes the modelling methodology, while the case descriptions of the DNS benchmark and the LH<sub>2</sub> tank are presented in Section 3. The 1D analysis of the K-Site LH<sub>2</sub> data is also included in this section. The results from the CFD simulations are presented and discussed in Section 4, before the main conclusions are drawn in Section 5.

## 2. Methodology

This section outlines the CFD methodology, including numerical setup and thermophysical properties, before

discussing buoyancy treatment in RANS models. The two simulation cases are presented in the following section.

### 2.1. Governing equations

The compressible Navier-Stokes equations are solved using OpenFOAM [28] (foundation, v12), with the *fluid* solver module.

The continuity equation reads,

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_j)}{\partial x_j} = 0 \quad (1)$$

where  $\rho = \rho(p, T)$  is the density which is obtained from an equation of state (EoS) and  $u_i$  is the  $i$ -th velocity component. The momentum balance equation reads

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \mu_{\text{eff}} \frac{\partial u_i}{\partial x_j} \right) - \frac{\partial p'}{\partial x_i} - g_j x_j \frac{\partial \rho}{\partial x_i}, \quad (2)$$

where  $p' = p - \rho g_j x_j$  is the *modified pressure*,  $g_i$  is the gravitational acceleration and  $\mu_{\text{eff}}$  is the effective viscosity (sum of molecular and turbulent contributions). The energy balance equation reads

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_j (h + K)}{\partial x_j} = - \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_j} \left( \alpha_{\text{eff}} \frac{\partial h}{\partial x_j} \right) + \rho u_i g_i, \quad (3)$$

where  $h$  is the specific enthalpy,  $K = \frac{1}{2} u_k u_k$  is the specific kinetic energy and  $\alpha_{\text{eff}}$  is the effective thermal diffusivity (sum of molecular and turbulent contributions). In Eqs. (1) to (3), Reynolds averaging is assumed, and the flow variables (e.g.  $\rho$ ,  $u_i$ ,  $p$ , and  $h$ ) represent Reynolds-averaged quantities.

Finally, the heat equation is also solved inside the tank wall,

$$\rho \frac{\partial e}{\partial t} = \frac{\partial}{\partial x_i} \left( \lambda(T) \frac{\partial T}{\partial x_i} \right), \quad (4)$$

where  $e = c_v(T) T$  is the specific internal energy and  $\lambda(T)$  the thermal conductivity. At fluid-solid interfaces, boundary conditions are specified by imposing energy conservation and continuity of temperature.

### 2.2. Equation of state and thermophysical properties

Previous CFD studies of LH<sub>2</sub> storage have commonly employed the ideal-gas equation of state (EoS) for the vapour phase, even though hydrogen exhibits significant real-gas effects under typical cryogenic storage conditions [29]. In the present work, the vapour phase is therefore modelled using the Peng–Robinson EoS [30], which offers improved accuracy in the relevant pressure and temperature range. Density predictions from the Peng–Robinson EoS and the ideal gas law are compared against the accurate reference multiparameter equation of state (MEOS) by Leachman et al. [31] for three different pressures in Fig. 1. The comparison shows that the Peng–Robinson

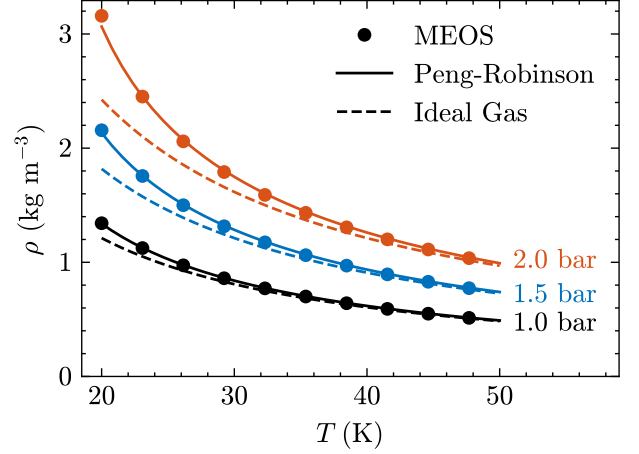


Figure 1: Density predictions of the Ideal Gas Law and Peng–Robinson EoS [30] (OpenFOAM implementation), compared with the MEOS by Leachman et al. [31].

EoS performs substantially better, particularly at lower temperatures, where real-gas effects are most pronounced. While the ideal-gas law exhibits density deviations of 9.5 % at 1.0 bar and up to 23.3 % at 2.0 bar, the Peng–Robinson model yields significantly smaller errors; only 0.39 % and 2.99 % at 1.0 bar and 2.0 bar, respectively.

The specific heat at constant pressure,  $c_p$ , is tabulated from NIST data for para-hydrogen [32], while thermal conductivity and dynamic viscosity are fitted as temperature polynomials to the same data.

In the liquid phase, temperature variations are significantly smaller than those occurring in the gas phase, and the resulting relative density changes are therefore small. For this reason, the Boussinesq approximation has been widely employed in previous studies [20, 17, 18]. In this work, the *rPolynomial* model in OpenFOAM is used, where the density  $\rho$  is given by

$$\frac{1}{\rho} = C_0 + C_1 T + C_2 T^2 - C_3 p - C_4 p T, \quad (5)$$

where the coefficients have been fitted to saturation conditions at 1 bar. Temperature polynomial fits are used for enthalpy, viscosity and thermal conductivity.

Without a catalyst, the conversion rate between para- and ortho-hydrogen is extremely slow. Petitpas et al. [33] found that para-ortho conversion required 10–15 days of dormancy to initiate and 25–30 days to complete conversion to the equilibrium composition. Since the K-Site experiments are of much shorter duration (less than 24 hours), para-ortho conversion effects are not considered in this work.

### 2.3. Turbulence modelling and the role of buoyancy

The flow in stationary cryogenic storage tanks is driven by density gradients caused by heat ingress from the tank

walls. This leads to the development of a natural convection boundary layer along the heated walls, which enhances heat transfer into the bulk fluid region. If the driving force is strong enough, the flow will eventually transition into a turbulent regime. This transition also depends on the geometry, and for cryogenic storage tanks, the vertical heated plate is often used as an approximation to judge whether the flow is expected to be laminar or turbulent.

A natural convection boundary layer on vertical flat plate with a fixed wall temperature transitions to turbulence when the Rayleigh number, defined as

$$\text{Ra} = \frac{\rho g \beta \Delta T L^3}{\mu \alpha}, \quad (6)$$

exceeds a critical value,  $\text{Ra}_c \approx 10^9$ . Here,  $g$  is the gravitational acceleration,  $\beta$  the thermal expansion coefficient,  $\Delta T = T_w - T_\infty$  the characteristic temperature difference,  $L$  the characteristic length, and  $\mu$  and  $\alpha$  the dynamic viscosity and thermal diffusivity, respectively. In this configuration, the plate has a constant temperature  $T_w$ , and  $T_\infty$  is the fluid's bulk temperature.

In the derivation of the transport equation for specific turbulent kinetic energy  $k$  with variable density, a *buoyancy production* term arises [34],

$$P_{b,k} = \overline{u'_i \rho'} g_i, \quad (7)$$

where  $u'_i$  and  $\rho'$  are the velocity and density fluctuations, respectively.

This term is included by default for selected turbulence models in some commercial solvers, but its inclusion is rarely reported in previous CFD studies of LH<sub>2</sub> storage tanks. As a result, its influence on predicted stratification, pressurization, and boil-off rate remains largely unexplored. In this work, the buoyancy source term is implemented in OpenFOAM as a run-time-selectable source term applicable to both the  $k$ - $\epsilon$  and  $k$ - $\omega$  turbulence model families.

The velocity-density correlation term in Eq. (7) is commonly modelled using the *Simple Gradient Diffusion Hypothesis* (SGDH) [34], using the turbulent Prandtl number  $\text{Pr}_t = \nu_t / \alpha_t$  (ratio of eddy viscosity and turbulent thermal diffusivity) and the Reynolds-averaged density gradient  $\partial \rho / \partial x_i$ . In this work,  $\text{Pr}_t = 0.85$  is adopted [10]. This leads to the following expression for the buoyancy source term:

$$P_{b,k} = \frac{\nu_t}{\text{Pr}_t} \frac{\partial \rho}{\partial x_i} g_i. \quad (8)$$

The buoyancy source term can act both as a source and a sink of turbulent kinetic energy, depending on the stratification. For stable stratification, the density decreases with vertical position,  $\nabla \rho \cdot \mathbf{g} > 0$ , which leads to  $P_{b,k} < 0$ . Thus, turbulent fluctuations are dampened by the stable stratification. On the other hand, unstable stratification has the heavier fluid on top,  $\nabla \rho \cdot \mathbf{g} < 0$ , which leads to  $P_{b,k} > 0$ . This enhances the turbulent fluctuations.

The source term is added semi-implicitly to the transport equation for  $k$ : for  $P_{b,k} > 0$  it is treated explicitly as a source term, whereas for  $P_{b,k} < 0$  it is linearized as  $(P_{b,k}^n / k^{n-1}) k^n$ , where  $n$  is the current time step. This treatment significantly improved robustness, particularly for low turbulence levels.

The source term is also added to the transport equation for turbulent dissipation rate as

$$P_{b,\epsilon} = C_{\epsilon 1} \tanh\left(\left|\frac{v}{u}\right|\right) \frac{\epsilon}{k} P_{b,k}, \quad (9)$$

where  $v$  and  $u$  are the velocity components parallel and normal to the gravitational acceleration, respectively, and  $C_{\epsilon 1}$  is a constant from the turbulence model. This term is also added semi-implicitly, but as it is already linear in  $\epsilon$ , the linearization procedure that was used for  $k$  is not needed.

The tanh limiter in Eq. (9) was proposed by Henkes et al. [35] and is widely used in the literature and in commercial codes [36, 37]. It acts as a limiter for  $P_{b,\epsilon}$ , which goes towards zero when the mean flow is horizontal (normal to the gravitational acceleration). However, Sebilliau [34] reported poor performance of this treatment of the buoyancy production term in the  $\epsilon$  equation in the context of Reynolds stress models and advised against its use. In the present work, omitting the limiter resulted in increased dissipation rates and reduced effective heat transfer relative to the DNS data, and it is therefore retained here.

In the  $k$ - $\omega$  SST model [25],  $P_b$  is also added to the transport equation for the specific dissipation rate  $\omega$ . Since it is already in linear form, it is treated implicitly as

$$P_{b,\omega} = \gamma \frac{\omega}{k} P_{b,k}, \quad (10)$$

where  $\gamma = 0.56$  [38].

For the  $v^2$ - $f$  model, the source term  $P_{b,v^2}$  is added to the transport equation for  $v^2$  in the same manner as the shear production term  $P_k$ . The effect of this source term is assessed using a benchmark case in Section 3.1.

#### 2.4. Solution algorithm

The fluid solver module in OpenFOAM is a so-called *all-Mach* solver, capable of modelling a compressible fluid at low Mach numbers without the time-step being constrained by the sound speed [39]. This makes it ideal for flows with low momentum but large density gradients due to temperature variations.

The PIMPLE algorithm is used for pressure-velocity coupling, which is a combination of the PISO (Pressure-Implicit with Splitting of Operators) [40] and SIMPLE (Semi-Implicit Method for Pressure Linked Equations) [41] algorithms. In each time step, a series of outer corrector iterations (PIMPLE loops) is performed, during which the gas, liquid, and metal regions are solved sequentially. A maximum of five outer correctors is allowed per time step; however, the PIMPLE loop is terminated early when

the initial pressure residual falls below  $10^{-3}$ . For simulations with the  $v^2 - f$  turbulence model [42], a tolerance of  $5 \times 10^{-3}$  is also used for the elliptic equation for  $f$ . Each PIMPLE iteration includes three inner PISO correctors and one or two non-orthogonal correctors (depending on the mesh-quality). After the initial transient phase, convergence within each time step is typically achieved using two to three outer correctors.

Temporal discretisation is performed using a second-order implicit backward scheme. Convective terms are discretised using the bounded second-order *limitedLinear* scheme. Spatial gradients are evaluated using a point-based least-squares method, and full non-orthogonal correction is applied in the Laplacian operator discretisation. Adaptive time stepping is employed, maintaining a maximum Courant number of  $\text{Co}_{\text{max}} = 0.5$ .

### 3. Case definitions

In this section, the cases to be simulated are defined. First, a benchmark case is introduced to assess the performance of different turbulence models against DNS data for a square cavity. After that, the sharp-interface formulation used to model pressurization and thermal stratification in the K-Site LH<sub>2</sub> tank is described. The corresponding results are presented in the following section and compared with experimental data.

#### 3.1. Benchmark case: The differentially heated square cavity

To evaluate the performance of the turbulence models for simulating natural convection at high Ra, a direct numerical simulation (DNS) dataset of turbulent natural convection in a differentially heated square cavity (DHSC) is employed as a benchmark reference, see [27]. We test a selection of three turbulence models, in addition to assessing the effect of adding the buoyancy production term  $P_b$ .

The 2D computational domain of the DHSC is illustrated in Fig. 2. The left and right vertical walls are hot and cold, respectively, while the top and bottom walls vary linearly from  $T_h$  to  $T_c$  from left to right. For consistency with the model used in the DNS dataset, the Boussinesq approximation is used for the buoyancy force in the momentum equations. We chose  $T_h = 50^\circ\text{C}$  and  $T_c = 10^\circ\text{C}$ , based on the experiments by [43]. Ra, which was defined in Eq. (6), is then modified by adjusting the length  $L$ . The DNS dataset contains simulation results for Ra ranging from  $10^8$  to  $10^{11}$ , and due to the application to LH<sub>2</sub> storage tanks, we use the two highest Ra cases, namely  $\text{Ra} = 10^{10}$  and  $\text{Ra} = 10^{11}$ .

In contrast to pressure-driven flows, where the logarithmic law of the wall is well known, the directional dependency of a natural convection boundary layer has made the development of universal wall functions challenging [27]. To accurately capture the viscous and thermal boundary

layers, the boundary layer is therefore often resolved in natural convection flows. This imposes higher-resolution requirements in both space and time, making transient simulations computationally intensive, even in two dimensions.

The alternative is to sacrifice accuracy for computational speed-up, and employ standard wall functions to avoid resolving the boundary layer. In natural convection flows, satisfying the conventional requirement  $30 < y^+ < 200$  can be problematic. The dominating velocity and temperature gradients are typically confined to the near-wall boundary layer, which may lie entirely below  $y^+ = 30$  in weakly turbulent flows. Enforcing  $y^+ > 30$  can therefore place the first computational cell centre outside the boundary layer and into the stagnant core region. For this reason, we use the *nutUSpaldingWallFunction* for  $\nu_t$ , which transitions smoothly from the log-law region to the viscous sublayer.

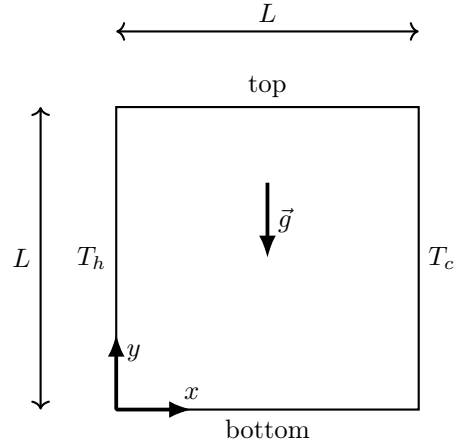


Figure 2: Domain and boundary conditions for the differentially heated square cavity ( $L \times L$ ) test case.

The heat transfer from the vertical walls is quantified by the average Nusselt number, defined as

$$\overline{\text{Nu}}_j = -\frac{1}{\Delta T} \int_0^L \frac{\partial T}{\partial x} \Big|_{x=x_j} dy \quad (11)$$

where  $j \in \{\text{hot}, \text{cold}\}$ ,  $x_{\text{hot}} = 0$  and  $x_{\text{cold}} = L$ .

To save computational time, a precursor simulation is performed using the  $v^2 - f$  model, and is used as the initial condition for all subsequent simulations. The simulations are run for  $t^* = 200$  before time averaging starts and they are then run for another  $t^* = 200$ . Here  $t^* = t\sqrt{\text{Ra}\alpha}/L^2$  is the non-dimensional time. The grid resolution is  $250 \times 250$  and  $300 \times 300$  for the  $\text{Ra} = 10^{10}$  and  $\text{Ra} = 10^{11}$  simulations, respectively.

#### 3.2. The K-Site tank case

The K-Site experiments were reported by Hasan et al. [14], Van Dresar et al. [15]. The utilized tank is constructed of two ellipsoidal caps with major diameter of

2.2 m and a major to minor axis ratio of 1.2, which gives a volume of 4.89 m<sup>3</sup>. The tank is constructed of aluminium 2219-T62, and is milled to a wall thickness of 2.08 mm. The thickness is increased near weld lands and the lid, although these variations are not specified in detail. The tank was instrumented with temperature sensors in the fluid and on the outside of the tank wall. The tank pressure was monitored in a closed configuration (pressurization tests) and the flow rate was measured in a vented configuration to estimate the average heat flux from the ambient (boil-off tests). Three different ambient temperatures were used to vary the heat ingress, and in this work we use the experiments with  $q_w = 3.5 \text{ W m}^{-2}$  average heat flux. Heat leaks through struts, piping, and instrumentation were also estimated in boil-off tests by Stochl and Knoll [13], and accounted for around 15 % of the total heat transfer rate of 49 W.

### 3.2.1. Analysis of experimental data

For the 83 % and 49 % fill levels, time series for the tank pressure and the thermocouples are available, sampled at 1/2 hour intervals. This allows for direct comparison of the temperature profiles and tank pressurization, and has been useful when validating both nodal and CFD models. This direct comparison does not, however, yield insight into the accuracy of the predicted mass transfer rate, which is of key interest when determining the accuracy of heat transfer correlations used at the interface.

In this section, the experimental data are used to estimate the evaporation rate and the mechanisms of pressurization. To estimate the evaporation rate, the mass of the vapour phase is calculated using temperature and pressure data. The key assumptions in this analysis are

1. The temperature only varies in the vertical direction, i.e., is uniform in the radial and azimuthal direction.
2. Hydrostatic and inertial pressure effects in the ullage are negligible compared with the total pressure in the tank.

With these assumptions, the experimental temperature data can be used to generate continuous temperature profiles at each sampled time. Together with the pressure, the total vapour mass in the ullage can readily be estimated as

$$m = \int_{y_{\text{interface}}}^{y_{\text{top}}} \rho(T(y), p) A_c(y) dy, \quad (12)$$

where  $A_c(y)$  is the cross sectional area at height  $y$ . Here, the vapour density  $\rho(T, p)$  is evaluated using the MEOS by Leachman et al. [31], and integration is performed with the trapezoid rule in *numpy*. This is done at each sampled time, and the boil-off rate is then estimated as the time derivative of the vapour mass,  $\dot{m}(t)$ .

In addition to estimating the boil-off rate, we also analysed the pressurization rate by decomposing it into thermal and boil-off-induced pressurization, analogously to the approach in [44]. Based on their findings, one can assume

that the velocities in the ullage are so low that inertial effects on pressure are negligible. The total time derivative of pressure is then expressed as

$$\begin{aligned} \frac{dp(y, t)}{dt} &= \left( \frac{\partial p}{\partial T} \right)_\rho \frac{dT(y, t)}{dt} + \left( \frac{\partial p}{\partial \rho} \right)_T \frac{d\rho(y, t)}{dt} \\ &= \Delta p_T(y, t) + \Delta p_{\dot{m}}(y, t). \end{aligned} \quad (13)$$

Here, we also assume that the pressure is uniform, and we calculate the terms by integrating over the volume

$$\begin{aligned} \Delta p_T &= \int \left( \frac{\partial p}{\partial T} \right)_\rho \frac{dT}{dt} A_c(y) dy \\ \Delta p_{\dot{m}} &= \int \left( \frac{\partial p}{\partial \rho} \right)_T \frac{d\rho}{dt} A_c(y) dy. \end{aligned} \quad (14)$$

This decomposition will reveal if either pressurization by thermal expansion or phase change (evaporation or condensation) dominates, which is useful when validating directly against the pressurization rate. To the authors' knowledge, this analysis has not been reported for this experiment before.

The resulting evaporation rate and pressurization components are shown in Fig. 3. From the boil-off rate, one can see that condensation occurs in the first 2 h to 3 h, before transitioning to net evaporation. This can also be seen from the pressurization components, where  $\Delta p_{\dot{m}}$  is negative. The thermal contribution  $\Delta p_T$  is positive and larger in magnitude than  $\Delta p_{\dot{m}}$ , so the net effect is a pressure increase, i.e., the heating of the gas compensates for the condensation. We also observe that  $\Delta p_T$  declines relatively fast and goes asymptotically to zero, whereas  $\Delta p_{\dot{m}}$  changes sign and accounts for pressurization alone after the initial transient. This indicates that the ullage is heated up significantly at the beginning of pressurization, but after around 5 h the thermal contribution is small. This means that the ullage does not become significantly warmer after this, and even more heat is available for evaporation of the liquid.

### 3.2.2. Boundary and initial conditions

The gas and liquid phases are modelled as separate single-phase regions, connected by a flat, stationary interface. In the following, the boundary conditions applied to all regions of the computational domain are described, including the coupling conditions imposed at the gas-liquid interface.

In the present work, the interface is explicitly resolved through the sharp-interface approach. We use the *quasi-equilibrium* phase change model, in which the heat fluxes are assumed to be sufficiently low for the interface to remain at the saturation temperature. In this limit, all heat transferred to the interface is directly used for phase change, eliminating the need for empirical coefficients. This contrasts with the Schrage phase-change model, which is derived from kinetic theory and permits  $T_i \neq T_{\text{sat}}$ . Kassemi et al. [20] compared both approaches and reported that

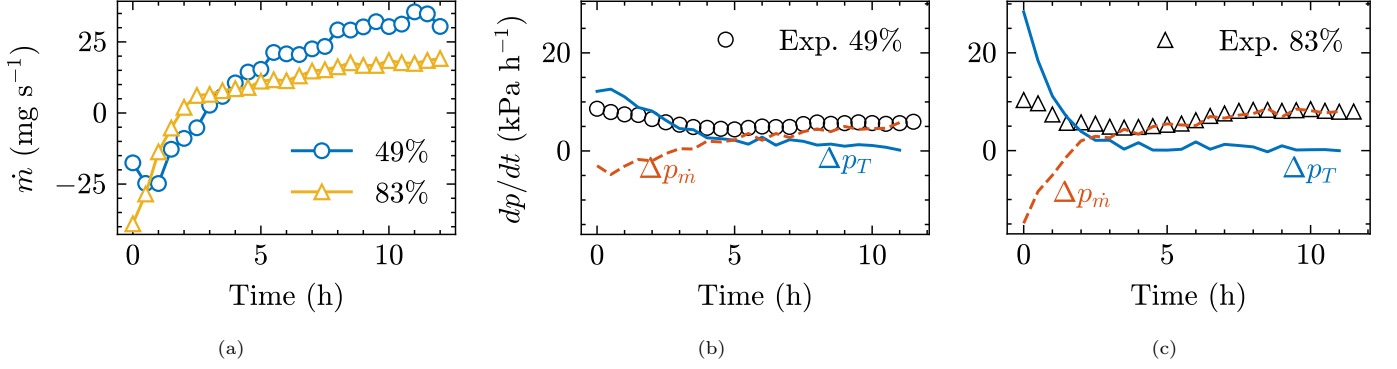


Figure 3: Results from the 1D analysis of the experimental K-Site data. (a) Estimated boil-off rate for 49 % and 83 % fill levels and pressurization decomposition for (b) 49 % fill level and (c) 83 % fill level.

they yield identical results under the conditions considered.

The thermal boundary condition of the interface is then

$$T_i = T_{\text{sat}}(p_{g,i}). \quad (15)$$

This condition is imposed as a Dirichlet boundary condition, with the interface temperature updated explicitly at each iteration using the current value of the gas-side interface pressure  $p_{g,i}$  in Eq. (15). The heat flux is evaluated at the interface as

$$q_{g,\ell \rightarrow \text{int}} = -\lambda_{\text{eff}} \left. \frac{\partial T}{\partial n} \right|_{g,\ell \rightarrow \text{int}}, \quad (16)$$

with  $\lambda_{\text{eff}}$  being the effective thermal conductivity at the interface. The mass flux from the liquid to the gas phase is then calculated as

$$m'' = \frac{q_{g \rightarrow \text{int}} + q_{\ell \rightarrow \text{int}}}{\Delta h_{\text{vap}}}, \quad (17)$$

where  $\Delta h_{\text{vap}}$  is the specific latent heat of vaporisation. The mass flux is translated to normal interface motion, but due to low mass fluxes, the interface normal movement is very small compared with the convective flows near the interface. Due to the large density ratio between the liquid and vapour phases, a given mass transfer results in a negligible change in liquid volume and mass [8]. In contrast, the vapour phase is highly compressible, such that the added mass directly influences the ullage pressure, while the liquid can be considered nearly incompressible under the present conditions. Consequently, the mass flux is applied only to the vapour side of the interface and not removed from the liquid, following the approach of Kassemi et al. [24],

$$u_{g,n} = \frac{m''}{\rho_g}, \quad u_{l,n} = 0. \quad (18)$$

For the tangential velocity component, the free surface condition holds on the interface between liquid and gas

$$u_{g,t} = u_{l,t} \quad \text{and} \quad \tau_g = \tau_l, \quad (19)$$

where  $u_{g,t}$  and  $u_{l,t}$  are the tangential interface velocity components in gas and liquid phases, respectively. The shear stress is defined as  $\tau = \partial u / \partial n \mu|_i$ .

For the turbulence quantities ( $k$ ,  $\epsilon$ ,  $\omega$ ,  $v^2$ ,  $f$ ,  $\nu_t$ ), standard wall treatment is used at tank walls, with wall functions being used on high-Re grids (where the boundary layer is not resolved), while for low-Re grids, low-Re boundary conditions are employed. On the gas side of the interface, the interface is treated as a wall for the turbulence quantities, while on the liquid side, zero-gradient boundary conditions are used [21]. All boundary conditions are summarized in Fig. 5.

The thermal boundary conditions on the outer side of the tank are also important, as they provide the driving force for flow and heat transfer within the tank. The heat transfer through the tank walls of the K-Site tanks was estimated in boil-off tests [13, 14, 15]. Most previous studies use a uniform heat flux boundary condition on the outside of the tank wall. Stewart and Moder [45] found that the variation in heat flux to the tank wall was less than 5 %. In a recent paper by Kartuzova et al. [17], the effect of a non-uniform heat distribution was demonstrated, where a fraction of the heat is diverted to the lid region of the boundary. This improved the predictions, and this approach will also be used here.

The initial temperature fields used for the three different fill levels are shown in Fig. 4. The fields are obtained by interpolating the experimentally measured temperatures from the K-Site experiments by Van Dresar et al. [15], Hasan et al. [14], where the *steady boil-off* initial condition was used. The liquid is initialised to the saturation temperature at the initial tank pressure  $p_0 = 1.03$  bar, which is justified by the fact that the tanks are initially vented, i.e., isobaric. Thus, at steady-state, the liquid will be close to saturation.

Before the start of the tank pressurization simulation, 30 minutes of isobaric flow is simulated in the liquid phase only (with the saturation temperature and a slip wall at the liquid-gas interface). Additionally, the energy equation is solved in the wall region, with Dirichlet boundary conditions at the gas boundary. This preconditioning al-

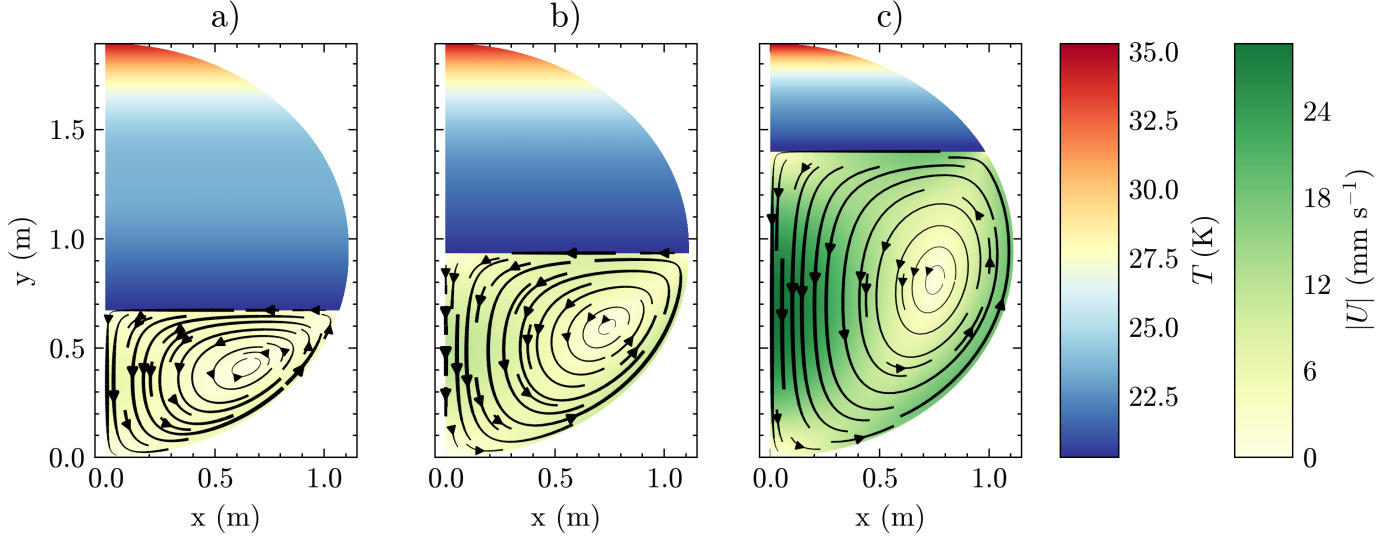


Figure 4: Initial velocity field in the liquid and temperature field in the gas for **a)** 29%, **b)** 49% and **c)** 83% fill levels. The temperature field is interpolated from experimental measurements [15], while the initial liquid velocity field is obtained by simulating only the liquid phase and solid regions for 30 min.

allows the liquid to develop a physically realistic natural convection pattern and avoids an artificially strong transient at early simulation times. The low-density gas phase is already stratified and reaches a developed flow state much faster than the liquid and was therefore not included in the preconditioning. The resulting initial liquid velocity fields and vapour temperature fields for the reference case at each fill level are shown in Fig. 4.

### 3.2.3. Numerical grid

The computational mesh is generated using *Gmsh* through a fully automated and parametrised scripting procedure. The simulations are performed on a two-dimensional axisymmetric grid, reducing the computational cost significantly compared with three-dimensional simulations. The mesh generation allows independent specification of the fill level, wall-normal ( $\Delta x_{w,n}$ ) and wall-tangential ( $\Delta x_{w,t}$ ) cell size, bulk cell size ( $\Delta x_b$ ), and boundary-layer growth rate. The grid is generated by using structured quad-blocks at the boundaries, connected by a quasi-structured quad-dominated grid in the bulk region. The wall-normal cell size grows with 5% per layer until it reaches the wall-tangential cell size. Additionally, variable wall thickness and internal wall boundaries can be added to the grid. At very high or very low fill levels, mesh skewness and non-orthogonality tend to increase because the liquid-gas interface is constrained to be horizontal, which can cause numerical stability issues. To mitigate this, a Laplacian smoothing procedure is applied after mesh generation. Assessment of the grid sensitivity of the model is presented in Appendix A. An illustration of the grid is shown in Fig. 6.

### 3.2.4. Modelling heat transfer in tank walls

Including the inner tank wall in the CFD model is essential, as heat transport from the dry to the wetted wall

region arises from the vertical temperature gradient, as demonstrated by several authors, e.g. Stewart and Moder [45], Kassemi and Kartuzova [46], Rossetti et al. [22].

The K-Site tank is made from milled AA2219 aluminium [13], with a thickness of 2.08 mm. The thermal conductivity and heat capacity in Eq. (4) exhibit significant variation in the temperature range relevant to this study for this alloy. Stewart and Moder [45] observed that the thermal conductivity of AA5083 closely resembles that of AA2219, and the NIST formulation for AA5083 was therefore adopted, as shown in Fig. 7a. In contrast, heat capacity (Fig. 7b) does not follow this correspondence: AA2219 aligns more closely with AA2024, while AA5083 deviates notably at low temperatures (4 K to 100 K), a discrepancy not addressed in previous K-Site tank simulations that employ the AA5083 alloy and one that will significantly affect thermal diffusivity. The tank alloy is tempered (T62), which tends to impact thermal conductivity in the cryogenic range [49]; however, data for this temper is not available, and we thus employ the available AA2219 (T81) data in this work.

In their recommendations for future work, Stewart and Moder [45] noted that the thermal contact resistance (TCR) between the tank and lid should be considered. To the authors' knowledge, this effect has not yet been included in existing CFD models, and its impact is investigated here. TCR depends on the materials in contact, surface roughness, contact pressure, and temperature. These details are not reported for the experiment considered, making specification challenging. While specific information on the K-Site lid attachment is unavailable, similar tanks commonly use indium wire as a sealant. Depending on the above factors, TCR can vary by orders of magnitude [50, 51]. In this work, two values are selected for the thermal contact con-

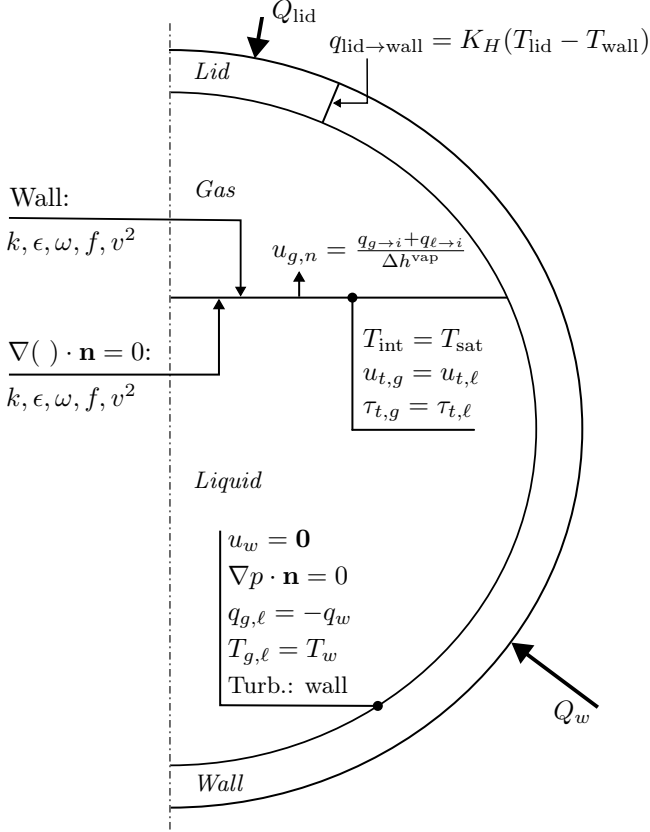


Figure 5: Overview of boundary conditions for the K-Site CFD model.

ductance (the inverse of the thermal contact resistance),  $K_H = 100 \text{ W m}^{-2} \text{ K}^{-1}$  and  $K_H = 1000 \text{ W m}^{-2} \text{ K}^{-1}$ , to cover a representative range of interface conditions. These values are chosen based on the measurements reported by Sunil Kumar and Ramamurthi [52], who found thermal contact conductances of this order of magnitude for aluminium joints over a range of contact pressures and temperatures between 50 K to 300 K.

### 3.2.5. Definition of reference cases

Two reference cases are defined to establish a consistent point of comparison for all simulations presented in this work. One for low-Re (wall resolved) grid labelled *LR*, and one for high-Re (wall modelled) grid labelled *HR*. The grid resolution is based on the results of the grid refinement analysis in Appendix A. The grids in the low-Re cases have  $\sim 170\,000$  cells, whereas the high-Re grids have  $\sim 52\,000$  cells. The reference case defined in Table 1 specifies the physical models, material properties, and boundary condition assumptions used throughout the study. The non-uniform heat flux is distributed such that 14% of the total heat (49.6 W [13]) is applied to the lid boundary, whereas the rest is distributed evenly on the rest of the tank wall.

The simulations require approximately 250 and 2000 CPU hours per simulated hour for the high-Re (HR) and low-Re (LR) reference cases, respectively. They were per-

formed on AMD EPYC Turin CPUs, using 32 cores for the HR case and 64 cores for the LR case. The significantly lower computational cost of the HR case is attributed to its coarser resolution near the wall, which also allows for larger time steps.

Table 1: Definition of the reference cases for low-Re (LR) and high-Re (HR) simulations.

| Parameter        | Low-Re                                | High-Re                               |
|------------------|---------------------------------------|---------------------------------------|
| RANS model       | $v^2 - f$                             | $k - \omega$ SST                      |
| $P_b$            | Enabled                               | Enabled                               |
| Tank material    | AA2219                                | AA2219                                |
| Wall thickness   | Constant                              | Constant                              |
| $q_w$            | Non-uniform                           | Non-uniform                           |
| $K_H$            | $100 \text{ W m}^{-2} \text{ K}^{-1}$ | $100 \text{ W m}^{-2} \text{ K}^{-1}$ |
| $\Delta x_{w,n}$ | 0.3 mm                                | 1.5 mm                                |
| $\Delta x_{w,t}$ | 2.0 mm                                | 4.0 mm                                |
| $\Delta x_b$     | 6.0 mm                                | 8.0 mm                                |

## 4. Results and Discussion

### 4.1. Benchmark case: The differentially heated square cavity

The local Nusselt number is shown in Fig. 8a for the cold wall. The laminar simulation is included as a reference, and under-predicts, as expected, the heat transfer in the cavity significantly.

Looking first at the performance of the different turbulence models *without* the buoyancy source term (dashed lines in Figs. 8a and 8b), it is clear that the  $v^2 - f$  and LS  $k - \epsilon$  models match the DNS results more closely than the  $k - \omega$  SST model. The LS  $k - \epsilon$  model matches quite well in the lower region of the cold wall, but under-predicts in the region close to the maximum Nu. The turbulent kinetic energy (TKE)  $k$  profile is sampled along the horizontal line  $y = L/2$ , and is compared against DNS data in Fig. 8b. It is evident that  $k - \omega$  SST under-predicts TKE in the boundary layer, both with and without the source term. LS  $k - \epsilon$  also under-predicts the peak TKE, but over-predicts the width of the turbulent boundary layer. This over-prediction is even more severe when including the source term. The  $v^2 - f$  model, on the other hand, closely matches the TKE profile. It slightly under-predicts close to the wall, but follows the DNS data closely, also in the transition to the laminar bulk region. It should also be noted that the LS  $k - \epsilon$  model failed to transition to turbulence when initialised from a quiescent initial condition, both with and without  $P_b$  and is hence not considered further in this work.

Also for the  $\text{Ra} = 10^{11}$  case, the  $v^2 - f$  model with  $P_b$  matches the DNS data closely, as can be seen in Fig. 9 (blue lines). To investigate the sensitivity to boundary layer resolution, the case is run with three different wall cell sizes  $\Delta x_w \in \{0.25 \times 10^{-3}, 1.0 \times 10^{-3}, 2.0 \times 10^{-3}\}$ , where

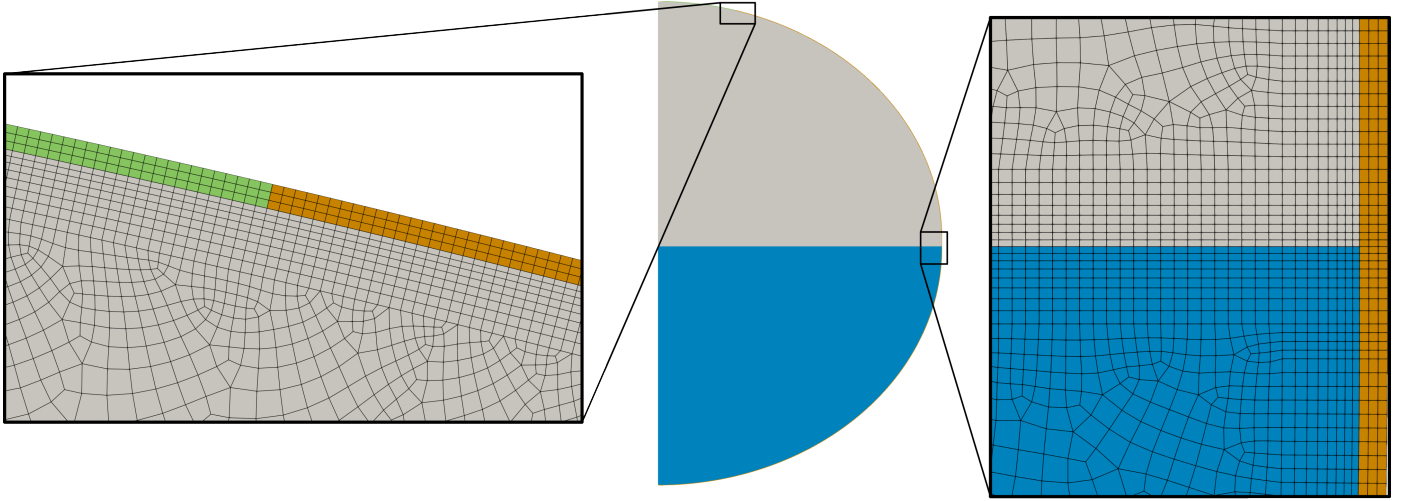


Figure 6: Illustration of numerical grid at 49 % fill level. The grid here is made coarser for illustrational purposes, and shows the structured boundary layer mesh at the wall, lid and interface boundaries, and the transition to the unstructured grid in the bulk fluid regions of the tank. The mesh regions are coloured: gas (grey), liquid (blue), tank wall (orange), and lid (green).

$\Delta x_w$  is the wall normal cell thickness normalized by the cavity length  $L$ . The bulk cell size and cell growth ratio are kept constant. These values resulted in  $y_{\max}^+$  of 1.29, 2.56 and 5.16, respectively. From Fig. 9b it is clear that the Nu profile shows asymptotic convergence, even with  $y_{\max}^+ > 1$ .

The results from using the  $k - \omega$  SST model with high-Re (wall function) treatment is also shown in Fig. 9 (yellow lines), with varying first wall cell size. In contrast to the wall-resolved  $v^2 - f$  simulations, no asymptotic convergence is observed with increased refinement of the wall cell height. The grid with  $\Delta x_w = 2.5 \times 10^{-3}$  matches the DNS data relatively well, but the finer ( $\Delta x_w = 1.25 \times 10^{-3}$ ) and coarser ( $\Delta x_w = 3.5 \times 10^{-3}$ ) grids both under-predict Nu in comparison (Fig. 9a). The same trend is seen in the TKE profile in Fig. 9b. This behaviour is likely a consequence of the fact that the wall functions are developed for pressure-driven boundary layers, which differ fundamentally from natural convection boundary layers that dominate here. The deviation from DNS data is still similar to what was observed in the  $Ra = 10^{10}$  case with a resolved boundary layer.

From these results, we conclude that the  $v^2 - f$  turbulence model on a wall resolved grid is the most accurate of the ones investigated here. Using the  $k - \omega$  SST turbulence model with wall functions introduces a modelling error that is sensitive to the wall-normal resolution. Therefore, a grid sensitivity analysis is required to ensure that this error does not significantly affect the results. For both the  $v^2 - f$  and  $k - \omega$  SST turbulence models, the impact of  $P_b$  is small for the DHSC case. Nevertheless, this term should be retained for physical consistency, as it may become more important in cryogenic fluids where density is more sensitive to temperature variations.

#### 4.2. The K-Site tank case

This section presents the simulation results from the K-Site tank. The focus is on the evolution of temperature, pressure and boil-off rate in the tank, and on the sensitivity of these responses to modelling choices. First, the effect of the buoyancy source term is presented, before impact of thermal boundary conditions, tank material and wall thickness are addressed.

##### 4.2.1. Impact of the buoyancy source term

This section will present and discuss the results from the simulations with (reference case) and without the buoyancy source term in the RANS models. The evolution of the tank pressure and the vertical temperature profile is shown in Fig. 10 for all three fill levels.

From the pressurization rates in Fig. 10, we see clearly that for all fill levels, the CFD model significantly underestimates when  $P_b$  is not accounted for (HR w/o  $P_b$  cases). For the 29 % and 83 % fill levels (Figs. 10a and 10c, respectively), the deviations are notable from early in the pressurization. On the other hand, it seems to be in closer agreement with the experiment for longer in the 49 % fill level. After around 7 h, however, the measured tank pressurization rate starts increasing. In contrast, the CFD simulation without  $P_b$  does not exhibit this increase, leading to larger deviations as the simulation progresses further.

For the CFD simulations *with*  $P_b$  (HR and LR reference cases), the pressurization predictions for the 29 % fill level are much closer to the experiments. We note that the HR and LR results are very similar initially, but the HR simulation begins to diverge from the LR case after approximately 5 h, predicting a slightly lower pressurization rate. The LR simulation remains closer to the experimental data. The simulations for the two highest fill levels (49 % and 83 %) also follow the experiments closely

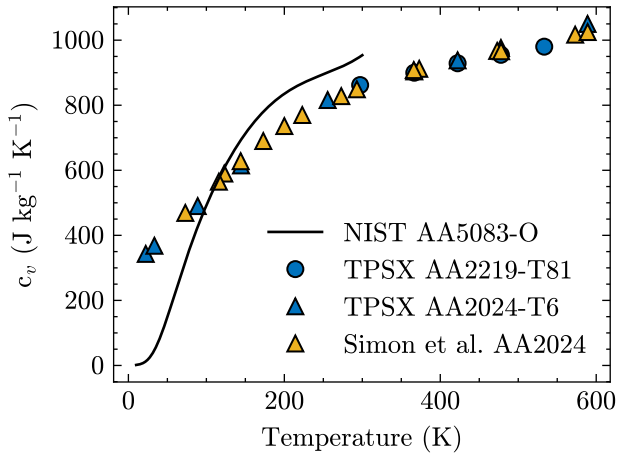
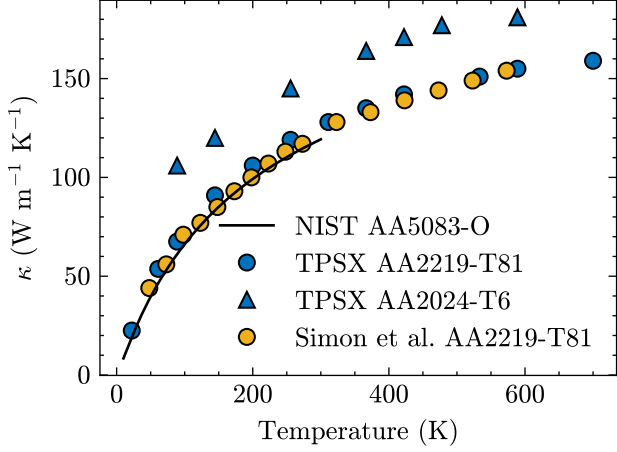


Figure 7: Thermal properties of aluminium alloys: (a) thermal conductivity and (b) specific heat capacity. Data from NIST [47], TPSX [48] and Simon et al. [49].

the first 2 h to 3 h. After this, the pressurization rate in the experiments decreases slightly before rising again to a quasi-steady state. This temporary dip in pressurization rate is not captured by the HR or LR reference cases, so the tank pressure is overestimated. After the pressurization rate stabilizes again, the HR simulation at 49 % fill level matches the experimental pressurization rate well, with a constant offset due to the temporary drop in pressurization rate. The same is true for the 83 % (Fig. 10c) fill level, but here the HR simulation quasi-steady pressurization rate is somewhat lower than that of the experiments.

Turning to the temperature profiles in Figs. 10d to 10f, the trend is clear: without  $P_b$ , the ullage stratification is significantly underpredicted at all fill levels. Here, stratification refers to the development of a vertical temperature gradient in the ullage, with warmer gas accumulating near the top and colder gas remaining near the liquid interface. This aligns with the observed pressurization behaviour, since the thermal contribution to pressure increase is smaller. On the other hand, the reference case

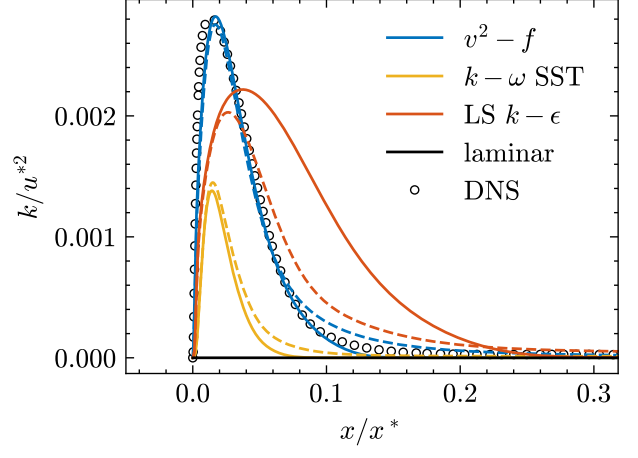
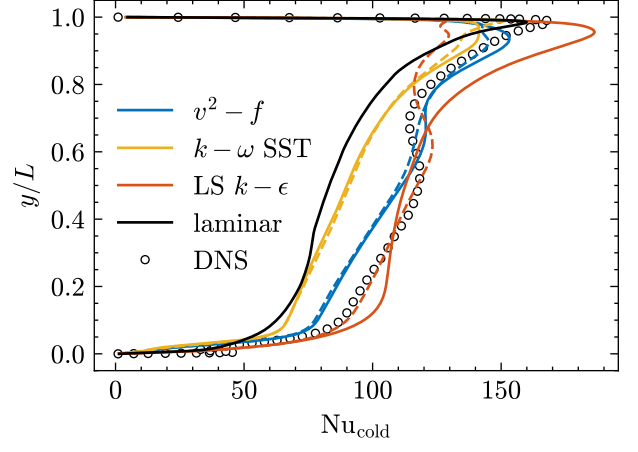


Figure 8: Results from the DHSC benchmark case, with  $Ra = 10^{10}$  with wall resolved (low-Re) grid, comparing turbulence models with (—) and without the buoyancy production source term  $P_b$  (---). (a) Time-averaged local Nusselt number distribution on cold wall and (b) time-averaged turbulent kinetic energy  $k$  normalized by the free fall velocity  $u^* = \alpha\sqrt{Ra}/L$  sampled at  $y = L/2$

simulations provide predictions much closer to the experiment for all fill levels. This is in contrast to the results in the DHSC (Fig. 9), where significant differences in heat transfer are observed for HR and LR treatment. In the DHSC configuration, the wall temperature was prescribed, whereas the  $LH_2$  tank is more representative of a fixed heat flux condition. The thermal resistance of the tank wall is small and identical in both the HR and LR simulations. Consequently, the total heat input to the vapour phase through the wall is essentially independent of the wall treatment. The primary region where differences between HR and LR could arise is therefore at the liquid boundary. However, when including  $P_b$ , both cases remain laminar in the vapour phase, such that the interfacial heat transfer is not influenced by the RANS modelling approach.

The impact of the buoyancy source term can be made clearer by examining the TKE in Fig. 11. The left-hand side of Figs. 11a and 11b shows the HR reference case

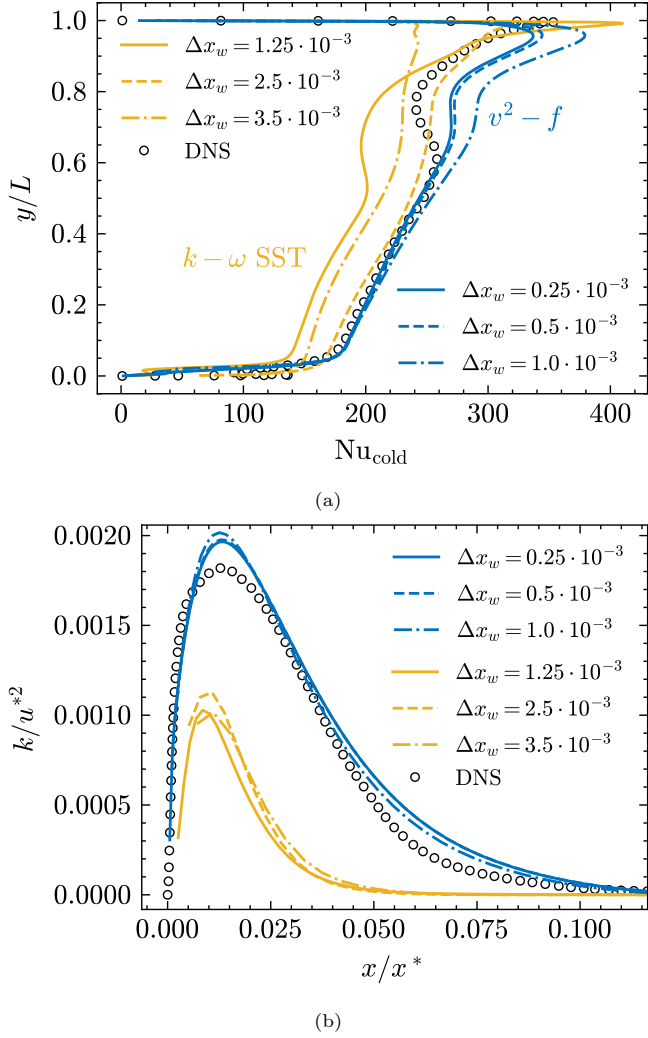


Figure 9: Results from the DHSC benchmark case, with different wall cell sizes for  $Ra = 10^{11}$ , using the  $v^2 - f$  model with low-Re treatment (blue) and the  $k - \omega$  SST model with high-Re treatment (yellow). Both use the buoyancy production source term  $P_b$ .

(with  $P_b$ ) for the 49% and 83% fill levels, respectively. Comparing the turbulence levels in the vapour phase, the differences observed in pressurization and stratification are linked to the role of  $P_b$ . In the reference cases, there is no turbulence in the vapour phase, while neglecting  $P_b$  predicts turbulence throughout the vapour region. This enhances mixing and increases the heat-transfer rate from the vapour to the liquid interface. As a result, the thermal stratification is significantly reduced compared with the experiments, see Figs. 10d to 10f. The same mechanism explains the lower predicted pressurization rates for simulations without  $P_b$ , since these are largely governed by thermal expansion. The liquid phase is also impacted by the buoyancy source term. When including the term (reference cases), the turbulence levels are elevated due to unstable stratification as a result of heating from below.

Compared with the predicted temperature profiles, the pressurization rate in Figs. 10a to 10c exhibits a larger dis-

crepancy between the HR and LR simulations. As shown in Section 3.2.1, the pressure rise results from both thermal expansion and boil-off effects, suggesting that the deviation primarily arises from differences in the predicted boil-off rate. The largest difference is observed at the 83% fill level, which is expected since the vapour volume is smallest in this case and therefore more strongly influenced by the boil-off gas.

The boil-off rate is shown in Figs. 13a and 13b for the 49% and 83% fill levels, respectively. They are compared with the estimated boil-off rates. To quantify the uncertainty arising from experimental temperature measurements, a Monte Carlo approach was employed. Gaussian noise with standard deviations of 0.3 K for wall temperatures and 0.05 K for fluid temperatures was added to the experimental data, and the boil-off estimation (Section 3.2.1) rate was recomputed for 1000 realizations. The resulting mean and standard deviation is shown in Figs. 13a and 13b with circular markers and error-bars, respectively. For both fill levels and all cases, the condensation from the CFD simulations in the first 2 h to 3 h is less than the experimental estimates. For the 49% fill level (Fig. 13a), the impact of  $P_b$  is also clear. After around 1 h the case without  $P_b$  transitions to net evaporation, whereas the reference case simulations transition to evaporation around the same time as the experiments ( $\sim 2.5$  h). At later simulation times, the HR and LR reference cases are in close agreement, with slightly higher boil-off rates predicted by the LR case, which is in accordance with the higher pressurization rate observed. The HR case without  $P_b$  is significantly higher, before being overtaken in boil-off rate by the HR reference case after around 10 h.

In the 83% fill level difference between the models is largest after the second half of the simulation, where the reference cases predict higher boil-off rates, with the LR simulation being closest to experimental estimates.

The initial discrepancies in boil-off rates may have several sources, including the sharp-interface assumption. This formulation constrains the interface by preventing any interface-normal motion except that associated with the prescribed phase-change velocity on the vapour side. Although these velocities are generally small, this restriction may influence convective mixing and thereby reduce the effective heat transfer at the interface.

The sharp-interface formulation also neglects capillarity-induced deformation of the interface near the tank wall and instead assumes that the flat interface extends directly to the wall. To assess the impact of this approximation, the equilibrium meniscus profile was estimated using the approach described in Appendix B. Using saturation properties for parahydrogen at 1 bar and a contact angle of  $\theta = 4^\circ$  [53], the predicted capillary rise at the wall (Eq. (B.2)) is 2.3 mm.

As shown in Fig. 12, the resulting area correction is significant only in a narrow region adjacent to the contact line, where  $(R_{int} - r)/R_{int} \lesssim 10^{-3}$ . Integrating the corrected mass flux over the interface (Eq. (B.4)) at the end

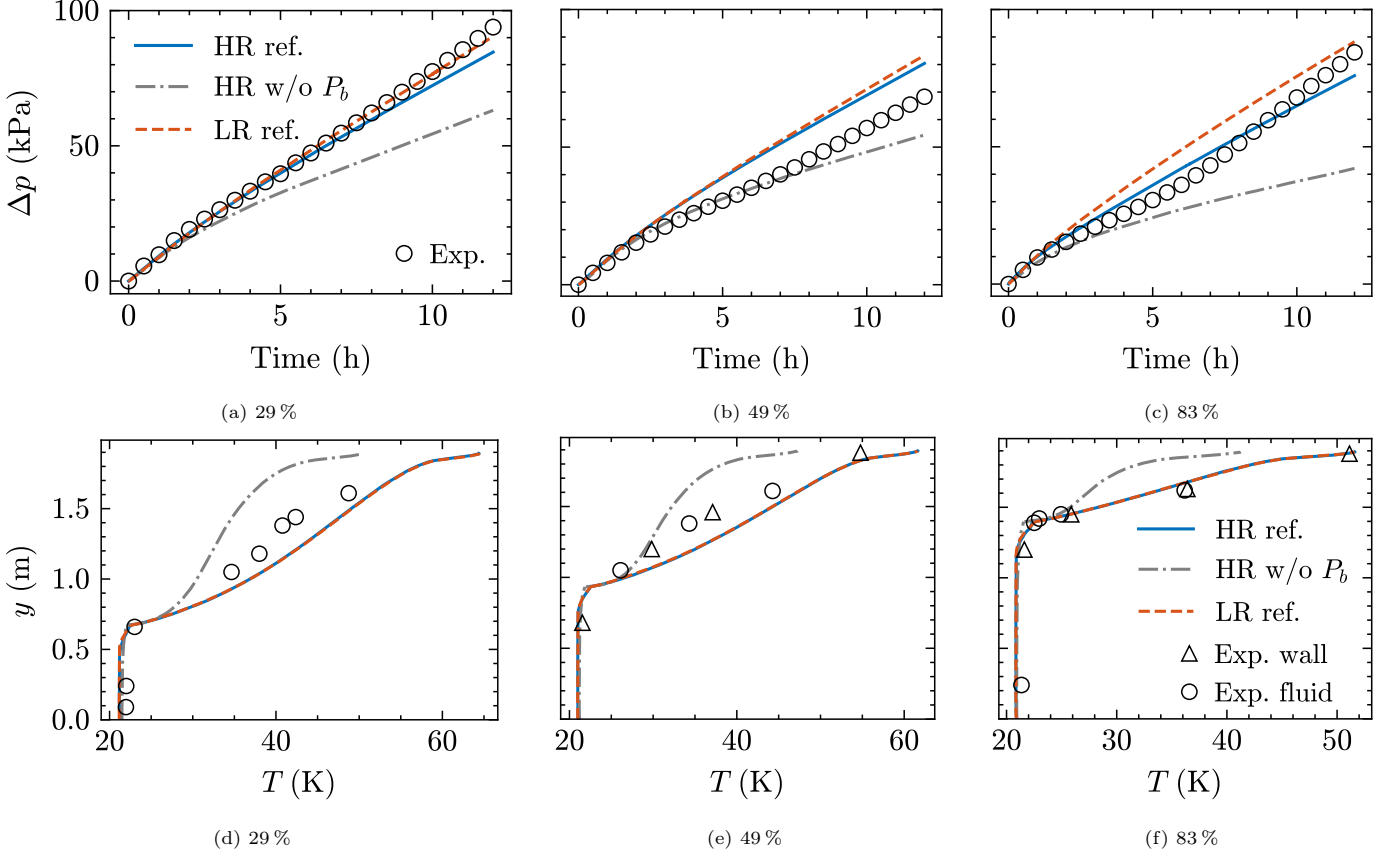


Figure 10: Pressurization results (a, b and c) and vertical temperature at  $t = 12$  h profile (d, e and f) evaluated at 6 h for the 29 % (a,d), 49 % (b,e) and 83 % (c,f) fill levels. The markers represent the values reported from the experiments, with measurement uncertainties of  $\pm 0.01$  kPa for pressure and  $\pm 0.1$  K and  $\pm 0.6$  K for the fluid and wall temperatures, respectively [14, 15].

of the simulation yields an increase in the estimated boil-off rate of only 1.39 % and 1.02 % for the 49 % and 83 % HR reference cases, respectively. For the corresponding LR reference cases, the estimated increase is substantially larger, at 18.01 % and 19.32 %.

This difference is attributed to the fact that the LR simulations resolve the thermal boundary layer near the contact line, leading to a more localized phase-change flux. Consequently, a larger fraction of the total boil-off originates from the region where the capillarity-induced area correction is largest.

These results suggest that neglecting the meniscus shape is unlikely to be a dominant source of the discrepancy between simulated and estimated boil-off rates in the HR reference cases. The larger corrections in the LR simulations indicate that capillarity becomes more relevant when phase change is strongly localized near the contact line, which is not captured in the HR grid. It should be noted, however, that the present estimate accounts only for the increase in interfacial area and assumes that the local mass flux remains unchanged. Furthermore, the analysis is based on a static contact angle of  $4^\circ$ , which is close to complete wetting and therefore produces a near-maximum capillary rise. Larger contact angles would result in a smaller meniscus and correspondingly smaller corrections.

#### 4.2.2. Impact of thermal boundary conditions

To assess the impact of the thermal boundary conditions, additional simulations are run using the HR reference case with variations in heat flux distribution and lid-tank thermal conductance  $K_H$ .

Fig. 14 shows the resulting temperature profiles for the 49 % fill level. The impact of increasing  $K_H$  by a factor of 10 is minimal, only reducing the outlet temperature at the top of the tank by around 2 K. On the other hand, enforcing a uniform heat flux  $q_w$  on the tank wall has a larger impact. This results in an outlet temperature that is more than 10 K lower than the reference case, with a decreasing difference also extending down towards the interface.

This illustrates that the effect of heat flux distribution on the tank wall is significant, and that prescribing accurate boundary conditions is important to correctly predict the tank behaviour.

#### 4.2.3. Impact of wall material and thickness

This section presents and discusses the impact of the tank material (Section 3.2.4) and wall thickness.

Using AA5083 instead of AA2219 leads to considerable overshoots of both stratification and pressurization, as is clear from Fig. 15. The main difference between the alloys is that the heat capacity of AA5083 is considerably lower

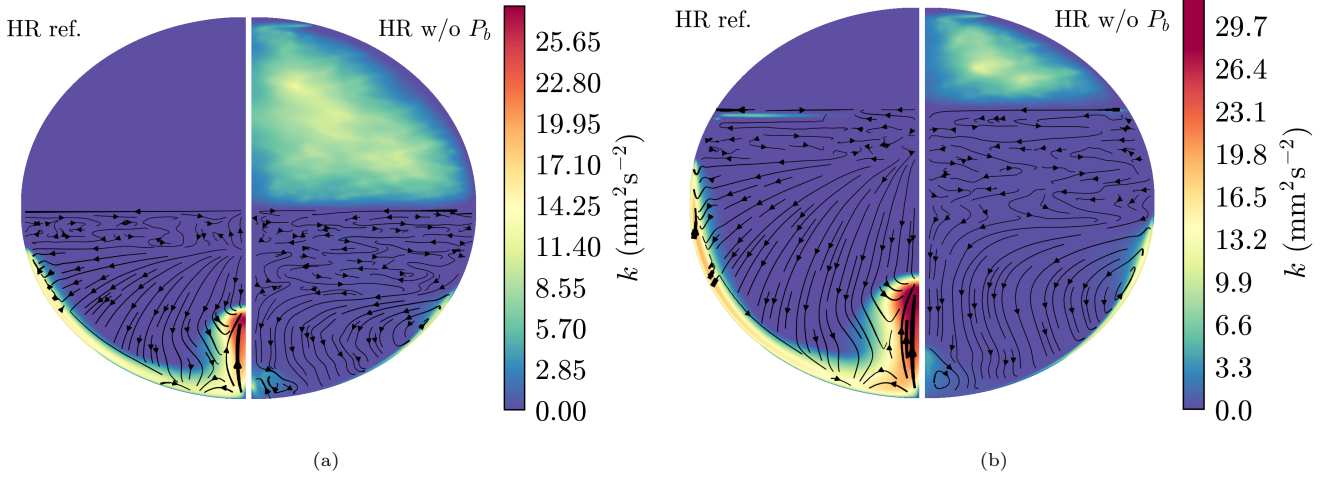


Figure 11: Comparison of time averaged (10 min) TKE and liquid streamlines for HR reference case and the HR case w/o buoyancy source term  $P_b$  for the a) 49 % fill level and (b) 83 % fill level.

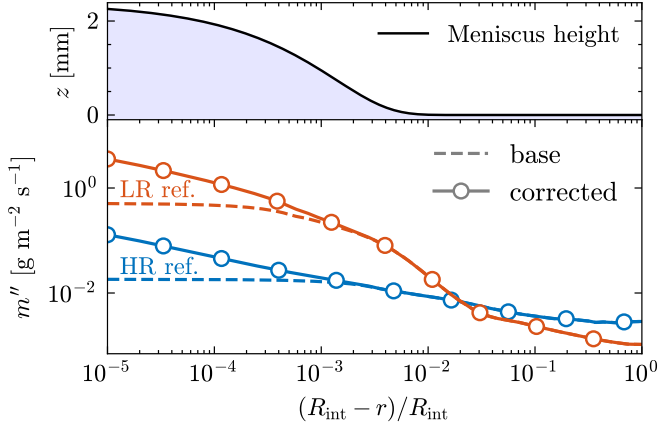


Figure 12: Impact of capillary area correction on the mass flux for the 83 % fill level HR and LR ref. cases at  $t = 12$  h. The interface height due to meniscus correction (Eq. (B.3)) is shown on the top.

(see Fig. 7b), which results in lower thermal mass and higher diffusivity. This leads to more of the heat being transferred directly to the ullage, whereas in the reference case, a larger fraction of the incoming heat contributes to heating tank material.

The boil-off rates are compared in Fig. 16a, and all cases except the AA5083 simulation are close to the reference case. In contrast to the pressurization rate and thermal stratification, the predicted boil-off rate from the AA5083 simulation shows closer agreement with the experimental estimate. This can be understood by considering the heat flux from the wall to the fluid near the interface, shown in Fig. 16b. The peak heat flux is observed just below the contact line, with the reference case reaching around  $40 \text{ W m}^{-2}$ . Using AA5083 increases the peak heat flux considerably, to  $65 \text{ W m}^{-2}$ . The same is true above the interface (in the ullage), even though the heat flux here is generally smaller. With the increase in heat input around the contact line, more heat is available for boil-off

generation, which is in accordance with the observations in Fig. 16a.

The variable wall thickness is achieved by adding extra wall material around weld lands, support structures, and around the lid, thereby increasing the thermal mass of the tank wall. Thus, the effect is the opposite of using AA5083, as the tank will absorb more heat during the thermal pressurization of the ullage. This leads to both reduced stratification and pressurization rate, in comparison with the reference case. As seen in Fig. 15a, the temperature profile is closer to the experimental reference everywhere except the uppermost sensor. The pressurization follows the experiments more closely, capturing the reduction of  $dp/dt$  in the early stages, while avoiding the under-prediction that occurred when not including the buoyancy source term.

#### 4.2.4. Sensitivity to heat flux distribution

To assess the impact of the assumed heat flux distribution on the predictions, an alternative distribution was tested in which only 75 % of the total heat enters the tank through the insulation and 25 % through the lid (compared with  $\sim 86$  % through the insulation in the reference case). This case is denoted HR var. wall 75 %  $Q_{MLI}$  in Figs. 15 and 16. For the 49 % fill level, this increase in lid heat flux predicts a top temperature that is much closer to what was achieved in the reference case with constant wall thickness (Fig. 15). The pressurization rate is also in closer agreement with experiment than the variable wall case with the reference heat flux distribution.

The same redistribution was also applied to the remaining two fill levels. As shown in Figs. 17 and 18, the redistribution improved predictions at the higher fill levels (49% and 83%) but degraded results at the lowest fill level (29%). It should be noted that the assumption of a time and fill level independent heat distribution is itself a simplification, since in reality the distribution is likely to

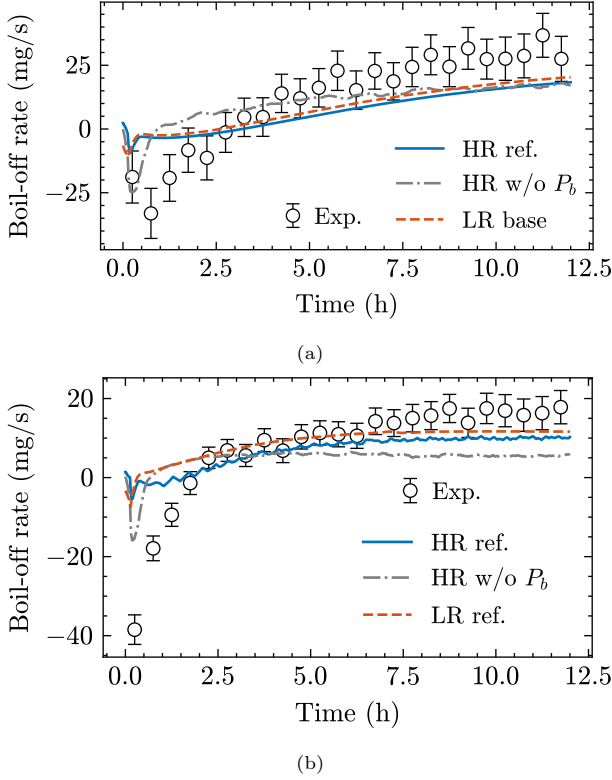


Figure 13: Boil-off rates for (a) 49% and (b) 83% fill levels. The CFD data has been filtered with rolling average with a 15 min window. The error bars represent uncertainty of boil-off estimate due to temperature measurement uncertainty ( $\pm\sigma$ ).

vary with both fill level and time. Indeed, the reference heat leak estimates [13] were performed for a tank at approximately 95% fill level operating at steady state, and may not be representative at lower fill levels and transient conditions. This may partly explain why the modified distribution improves some cases while deteriorating others.

Future work should therefore consider coupling the CFD model with a detailed thermal model of the tank structure and insulation to obtain a more realistic heat flux distribution.

## 5. Conclusions

In this work, a two-phase sharp-interface model for cryogenic storage tanks has been implemented in OpenFOAM. The model treats the liquid and ullage as single-phase regions coupled via interfacial boundary conditions, with the interface assumed to be at equilibrium. The existing turbulence models have been extended by adding a buoyancy source term  $P_b$  to transport equations for  $k$ ,  $v^2$ ,  $\omega$  and  $\epsilon$ , acting as a source or sink of turbulent kinetic energy, depending on the density stratification.

A DNS dataset of turbulent natural convection in a differentially heated square cavity was used to assess the predictive capability of the turbulence models and the influence of  $P_b$ . The  $v^2 - f$  model performed well at both Ra

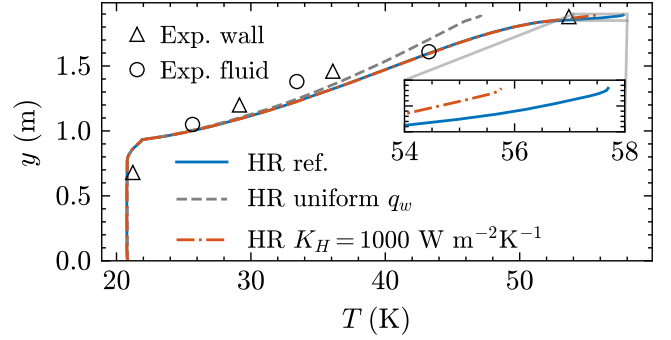


Figure 14: Temperature profile for high-Re cases, comparing the reference case with uniform wall heat flux  $q_w$  and increased  $K_H = 1000 \text{ W m}^{-2} \text{ K}^{-1}$ . Sampled at  $t = 8 \text{ h}$  and compared with experimental measurements.

investigated, whereas the  $k - \omega$  SST model underpredicted Nu. The effect of  $P_b$  was minor in these cases, but showed a more significant role under cryogenic conditions in the following analysis.

The sharp-interface model was used to simulate the K-Site experiments (4.89 m<sup>3</sup> spheroid LH<sub>2</sub> tank). Across all fill levels of the K-Site tank, the inclusion of the buoyancy production term led to a complete suppression of turbulence in the vapour region. Without this term, excessive turbulent mixing in the ullage resulted in an underprediction of both thermal stratification and pressurisation rate, consistent with observations reported in previous RANS-based studies of the same experiment. With the addition of this source term, the  $k - \omega$  SST model achieved reasonable agreement with experiments in predicting steady pressurisation rates and thermal stratification in the ullage across all fill levels.

In addition to validating against the reported measurements of temperature and pressure, we estimated the mass-transfer rate during the experiments using available data (for the two highest fill levels). These estimates allowed for direct comparison against the boil-off rate predicted by the CFD model, and revealed that the experiments exhibit condensation at the start of pressurisation, which is not fully captured by the CFD model. In general, the CFD simulations underpredicted the magnitude of the boil-off rate (both during condensation and evaporation), but captured the qualitative trend. Using the equilibrium meniscus profile to estimate the error associated with the flat-interface assumption at the wall, a quantitative analysis shows that this assumption contributes only marginally to the boil-off underprediction in the HR (high-Re) cases ( $\sim 1\%$ ), while a larger effect is observed in the LR (low-Re) simulations ( $\sim 20\%$ ) because a greater share of the mass transfer takes place near the wall, increasing sensitivity to interfacial area corrections near the contact line. A further analysis of the pressurisation mechanisms revealed that thermal expansion in the ullage is driving pressurisation during the first hours, before boil-off dominates. This enabled identifying the modelling errors that lead to dis-

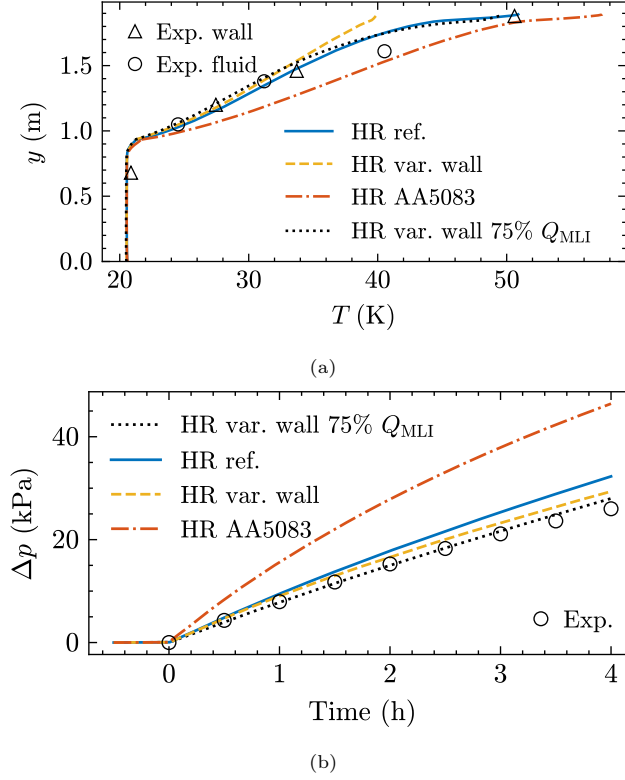


Figure 15: Impact of wall alloy, wall thickness and heat flux distribution at 49% fill level on (a) thermal stratification at  $t = 4$  h and (b) tank pressurization.

crepancies in pressurisation, allowing for targeted efforts in improving future CFD models.

The influence of the thermal boundary conditions at the tank wall was also investigated and found to be significant. The use of a non-uniform heat-flux distribution, together with thermal contact resistance at the lid-tank interface, improved the prediction of ullage temperatures in the upper region.

Accounting for variable wall thickness likewise had a distinct effect on the pressurisation rate, underscoring the importance of thermal mass. For future studies aiming to model a specific tank geometry with high fidelity, a more detailed representation of the tank structure and insulation should be included in order to provide more realistic thermal boundary conditions for the CFD model.

## Acknowledgements

This work was funded by the Research Council of Norway (project no. 342616). Furthermore, the following parties are also acknowledged for financial support: Gassco, Equinor, Air Liquide, HD Korea Shipbuilding & Offshore Engineering, Moss Maritime and the Research Council of Norway (project no. 320233). The simulations were performed on resources provided by Sigma2 - the National Infrastructure for High-Performance Computing and Data Storage in Norway. We gratefully acknowledge Rémi Manceau

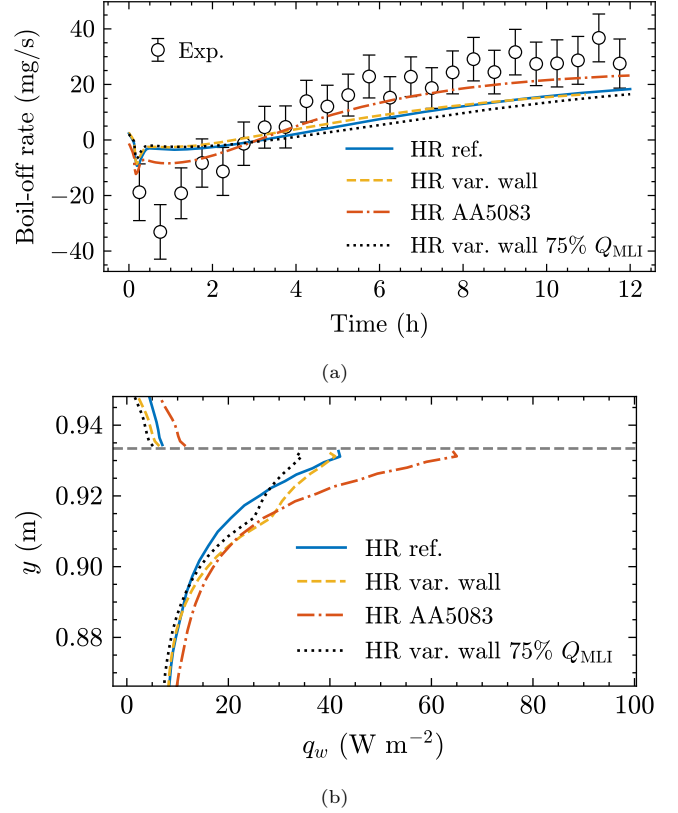


Figure 16: Impact of wall alloy, wall thickness and heat flux distribution at 49% fill level on (a) Boil-off rate and (b) time averaged (10 min) heat flux  $q_w$  at the wall-fluid boundary, sampled at  $t = 4$  h. The dashed line is the interface position.

for sharing the DNS dataset for the differentially heated square cavity.

## CRedit authorship contribution statement

**Johan R. Espelund:** Conceptualization, Methodology, Software, Visualization, Writing - Original Draft  
**Åsmund Ervik:** Supervision, Conceptualization, Writing - Review & Editing  
**Svend Tollak Munkejord:** Supervision, Conceptualization, Writing - Review & Editing  
**Magnus Aa. Gjennestad:** Methodology, Writing - Review & Editing  
**Luca Brandt:** Supervision, Conceptualization, Writing - Review & Editing  
**Corinna Schulze-Netzer:** Supervision, Conceptualization, Writing - Review & Editing

## Appendix A. Grid sensitivity analysis

To assess the grid sensitivity of the model, three different grids were considered. All grid parameters (wall normal, wall tangential and bulk cell sizes) are scaled by a factor 2 and  $1/2$  to obtain the coarse and fine grids, respectively. Otherwise, all parameters are kept constant and equal to the base-case specification in Table 1.

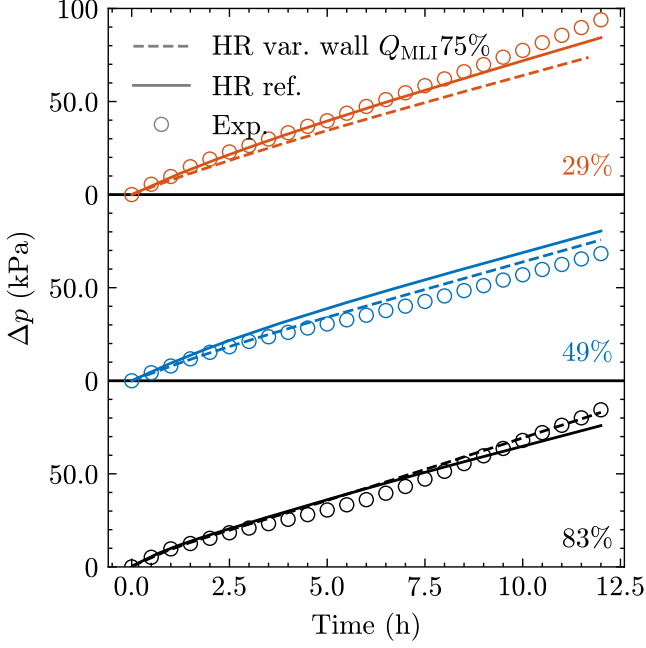


Figure 17: Comparison of pressurization rate between HR reference case and variable wall with redistributed heat flux, for all fill levels.

The initial state is quiescent, and the simulations are run for a simulated time of  $t_{\text{end}} = 10$  minutes. To assess grid convergence, the average pressurization rate is used,

$$\Phi = \frac{1}{(t_{\text{end}} - t_{\text{start}})^2} \int_{t_{\text{start}}}^{t_{\text{end}}} p_{i,v}(t) dt, \quad (\text{A.1})$$

where  $t_{\text{start}} = 0$  and  $t_{\text{end}} = 10$  min. The results are shown in Fig. A.19, and shows that for both the high-Re and low-Re grids, the medium grid resolution (the one used in the base-cases) is in the asymptotic range. The deviations from the Richardson extrapolate is less than 1% and 0.4% for the high-Re and low-Re medium grids, respectively.

## Appendix B. Meniscus correction to interfacial boil-off estimate

To estimate the effect of neglecting the meniscus shape of the liquid-vapour interface near the tank wall, an analytical equilibrium solution for a meniscus adjacent to a vertical wall is used [54]. This provides an order-of-magnitude estimate of the additional interfacial area associated with the curved interface near the equilibrium contact line.

The capillary length is defined as

$$L_c = \sqrt{\frac{\sigma}{\Delta\rho g}}, \quad \Delta\rho = \rho_\ell - \rho_v, \quad (\text{B.1})$$

where the surface tension  $\sigma = 1.937 \times 10^{-3} \text{ N m}^{-1}$  for para-hydrogen at 1.0 bar [32]. For a vertical wall with

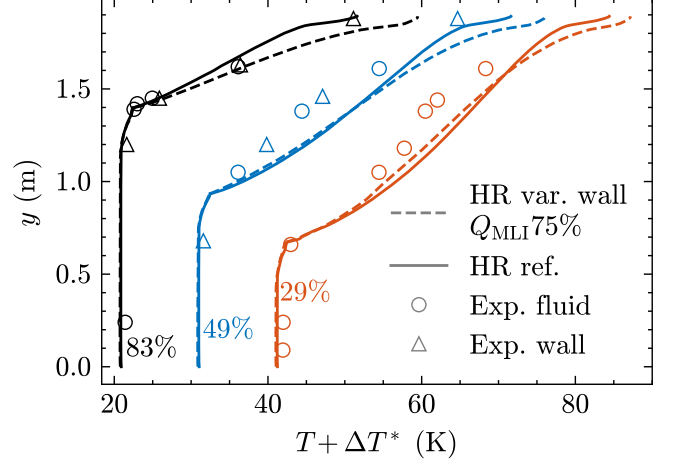


Figure 18: Stratification for all fill levels at  $t = 12$  h. For visualisation, the 49% and 29% profiles are offset with  $\Delta T^* = 10$  K and 20 K, respectively.

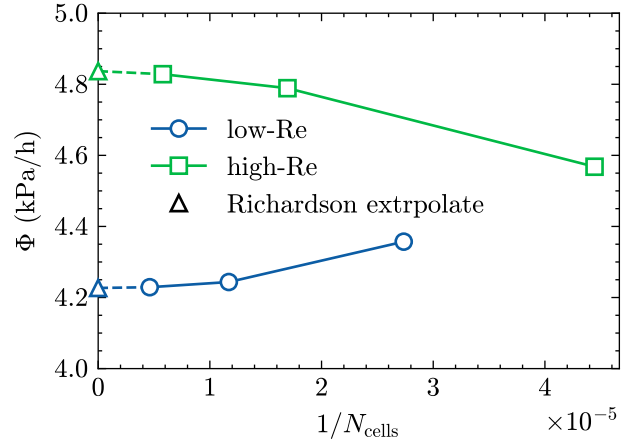


Figure A.19: Grid convergence for the low-Re and high-Re base cases, with the Richardson extrapolate of the mean pressurization rate  $\Phi$ .

equilibrium contact angle  $\theta$ , the corresponding capillary rise at the wall is given by

$$z_0 = \sqrt{\frac{2\sigma(1 - \sin\theta)}{\Delta\rho g}}. \quad (\text{B.2})$$

The equilibrium meniscus profile provides the interface height  $z$  as a function of the wall-normal distance  $x$  from the contact line,

$$\frac{x}{L_c} = \cosh^{-1}\left(\frac{2L_c}{z}\right) - \cosh^{-1}\left(\frac{2L_c}{z_0}\right) + \sqrt{4 + \frac{z_0^2}{L_c^2}} - \sqrt{4 + \frac{z^2}{L_c^2}}. \quad (\text{B.3})$$

The profile is evaluated using saturation properties for parahydrogen at 1 bar and a contact angle of  $\theta = 4^\circ$  [53].

The meniscus profile obtained from Eq. (B.3) is used to estimate the increase in interfacial area near the contact line. Assuming that the local mass flux  $m''(r)$  remains

unchanged, the corrected boil-off rate is calculated by integrating the simulated mass flux over the modified interface area,

$$\dot{m}_{\text{corr}} = 2\pi \int_0^{R_{\text{int}}} m''(r) \sqrt{1 + \left(\frac{dz}{dr}\right)^2} r dr. \quad (\text{B.4})$$

## References

- [1] M. van der Spek, C. Banet, C. Bauer, P. Gabrielli, W. Goldthorpe, M. Mazzotti, S. T. Munkejord, N. A. Røkke, N. Shah, N. Sunny, D. Sutter, J. M. Trusler, M. Gazzani, Perspective on the hydrogen economy as a pathway to reach net-zero CO<sub>2</sub> emissions in Europe, *Energy & Environmental Science* 15 (2022) 1034–1077. doi:10.1039/D1EE02118D.
- [2] R. R. Ratnakar, N. Gupta, K. Zhang, C. Van Doorne, J. Fesmire, B. Dindoruk, V. Balakotaiah, Hydrogen supply chain and challenges in large-scale LH<sub>2</sub> storage and transportation, *International Journal of Hydrogen Energy* 46 (2021) 24149–24168. doi:10.1016/j.ijhydene.2021.05.025.
- [3] K. I. Matveev, J. W. Leachman, The Effect of Liquid Hydrogen Tank Size on Self-Pressurization and Constant-Pressure Venting, *Hydrogen* 4 (2023) 444–455. doi:10.3390/hydrogen4030030.
- [4] E. Lan, S. Shi, W. Ji, M. Ishii, Modeling and simulation of cryogenic propellant tank pressurization in normal gravity, *Applied Thermal Engineering* 236 (2024) 121628. doi:10.1016/j.applthermaleng.2023.121628.
- [5] L. M. Claussner, G. E. Scarponi, F. Ustolin, Thermo-Fluid Dynamics Modelling of Liquid Hydrogen Storage and Transfer Processes, *Hydrogen* 6 (2025) 122. doi:10.3390/hydrogen6040122.
- [6] H. D. N. Nuwantha, D. Jung, C. Huh, Improvement in predicting the thermal behavior of liquid hydrogen storage through novel thermal modeling, *International Journal of Hydrogen Energy* 72 (2024) 1143–1158. doi:10.1016/j.ijhydene.2024.05.382.
- [7] S. Z. S. Al Ghafri, A. Swanger, V. Jusko, A. Siahvashi, F. Perez, M. L. Johns, E. F. May, Modelling of Liquid Hydrogen Boil-Off, *Energies* 15 (2022) 1149. doi:10.3390/en15031149.
- [8] S. Barsi, M. Kassemi, Numerical and experimental comparisons of the self-pressurization behavior of an LH<sub>2</sub> tank in normal gravity, *Cryogenics* 48 (2008) 122–129. doi:10.1016/j.cryogenics.2008.01.003.
- [9] F. Huerta, V. Vesovic, CFD modelling of the isobaric evaporation of cryogenic liquids in storage tanks, *International Journal of Heat and Mass Transfer* 176 (2021) 121419. doi:10.1016/j.ijheatmasstransfer.2021.121419.
- [10] F. Huerta, V. Vesovic, CFD modelling of the non-isobaric evaporation of cryogenic liquids in storage tanks, *Applied Energy* 356 (2024) 122420. doi:10.1016/j.apenergy.2023.122420.
- [11] K. I. Matveev, J. W. Leachman, Modeling of Liquid Hydrogen Tank Cooled with Para-Orthohydrogen Conversion, *Hydrogen* 4 (2023) 146–153. doi:10.3390/hydrogen4010010.
- [12] H. Wang, B. Wang, J. Sun, Q. Pan, G. Luo, X. Tao, Y. He, J. Pfothner, T. Jin, Z. Gan, Experimental and computational fluid dynamic investigation on thermal behaviors of liquid hydrogen during the no-vented storage process: A literature review, *International Journal of Hydrogen Energy* 57 (2024) 822–843. doi:10.1016/j.ijhydene.2024.01.062.
- [13] R. J. Stochl, R. H. Knoll, Thermal performance of a liquid hydrogen tank multilayer insulation system at warm boundary temperatures of 630, 530, and 152 R, in: *AIAA*, 1991.
- [14] M. M. Hasan, C. S. Lin, N. T. Vandresar, Self-pressurization of a flightweight liquid hydrogen storage tank subjected to low heat flux, in: 1991 ASME/AIChE National Heat Transfer Conference, Minneapolis, MN, 1991.
- [15] N. T. Van Dresar, M. M. Hasan, C.-S. Lin, Self-pressurization of a flightweight liquid hydrogen tank: Effects of fill level at low wall heat flux, in: *AIAA*, 1992.
- [16] S. Barsi, M. Kassemi, Investigation of Tank Pressurization and Pressure Control—Part I: Experimental Study, *Journal of Thermal Science and Engineering Applications* 5 (2013). doi:10.1115/1.4023891.
- [17] O. Kartuzova, M. Kassemi, D. Hauser, CFD validation of k-site tank self-pressurization under varying fill levels and heat fluxes with different turbulence models, *Cryogenics* 152 (2025) 104210. doi:10.1016/j.cryogenics.2025.104210.
- [18] S. Fernandes, E. Korsukova, C. Ellis, S. Ambrose, C. Eastwick, A CFD comparison of interfacial phase change models for boil-off, self-pressurisation and thermal stratification in liquid hydrogen storage tanks, *International Journal of Heat and Mass Transfer* 256 (2026) 128067. doi:10.1016/j.ijheatmasstransfer.2025.128067.
- [19] R. W. Schrage, A Theoretical Study of Interphase Mass Transfer, 1st ed ed., Columbia University Press, New York, NY, 1953.

- [20] M. Kassemi, O. Kartuzova, S. Hylton, Validation of two-phase CFD models for propellant tank self-pressurization: Crossing fluid types, scales, and gravity levels, *Cryogenics* 89 (2018) 1–15. doi:10.1016/j.cryogenics.2017.10.019.
- [21] C. Patel, H. Q. Yang, B. Williams, Validation of Gas-Liquid Sharp Interface Model in Loci-Stream for Propellant Tank Self-pressurization under Normal Gravity, in: *AIAA SCITECH 2024 Forum*, American Institute of Aeronautics and Astronautics, Orlando, FL, 2024. doi:10.2514/6.2024-0543.
- [22] F. Rossetti, M. Pizzarelli, R. C. Pellegrini, E. Cavallini, M. Bernardini, Setup of a numerical methodology for the study of self-pressurization of cryogenic tanks, *Cryogenics* 147 (2025) 104059. doi:10.1016/j.cryogenics.2025.104059.
- [23] F. Perez, S. Z. S. Al Ghafri, L. Gallagher, A. Siahvashi, Y. Ryu, S. Kim, S. G. Kim, M. L. Johns, E. F. May, Measurements of boil-off gas and stratification in cryogenic liquid nitrogen with implications for the storage and transport of liquefied natural gas, *Energy* 222 (2021) 119853. doi:10.1016/j.energy.2021.119853.
- [24] M. Kassemi, D. M. Hauser, O. V. Kartuzova, S. L. Hylton, Development and Validation of Two-Phase CFD Models for Key Elements of Propellant Tank CFM Operations in 1G and Microgravity – An Overview, in: *AIAA SCITECH 2023 Forum*, American Institute of Aeronautics and Astronautics, National Harbor, MD & Online, 2023. doi:10.2514/6.2023-1218.
- [25] F. Menter, M. Kuntz, R. B. Langtry, Ten years of industrial experience with the SST turbulence model, *Heat and Mass Transfer* 4 (2003).
- [26] O. V. Kartuzova, M. Kassemi, Validation of a Two-Phase CFD Model for Predicting Tank Self-Pressurization in the Ground-Based K-Site Experiment, in: *AIAA SCITECH 2025 Forum*, American Institute of Aeronautics and Astronautics, Orlando, FL, 2025. doi:10.2514/6.2025-0353.
- [27] F. Sebilliau, R. Issa, S. Lardeau, S. P. Walker, Direct Numerical Simulation of an air-filled differentially heated square cavity with Rayleigh numbers up to  $10^{11}$ , *International Journal of Heat and Mass Transfer* 123 (2018) 297–319. doi:10.1016/j.ijheatmasstransfer.2018.02.042.
- [28] H. G. Weller, G. Tabor, H. Jasak, C. Fureby, A tensorial approach to computational continuum mechanics using object-oriented techniques, *Computer in Physics* 12 (1998) 620–631. doi:10.1063/1.168744.
- [29] A. Aasen, M. Hammer, S. Lasala, J.-N. Jaubert, Ø. Wilhelmsen, Accurate quantum-corrected cubic equations of state for helium, neon, hydrogen, deuterium and their mixtures, *Fluid Phase Equilibria* 524 (2020) 112790. doi:10.1016/j.fluid.2020.112790.
- [30] D.-Y. Peng, D. B. Robinson, A New Two-Constant Equation of State, *Industrial & Engineering Chemistry Fundamentals* 15 (1976) 59–64. doi:10.1021/i160057a011.
- [31] J. W. Leachman, R. T. Jacobsen, S. G. Penoncello, E. W. Lemmon, Fundamental Equations of State for Parahydrogen, Normal Hydrogen, and Orthohydrogen, *Journal of Physical and Chemical Reference Data* 38 (2009) 721–748. doi:10.1063/1.3160306.
- [32] E. W. Lemmon, M. O. McLinden, D. G. Friend, Thermophysical properties of fluid systems, in: P. J. Linstrom, W. G. Mallard (Eds.), *NIST Chemistry Webbook, NIST Standard Reference Database*, volume 69, National Institute of Standards and Technology, Gaithersburg MD, 20899, USA, 1998.
- [33] G. Petitpas, S. M. Aceves, M. J. Matthews, J. R. Smith, Para-H<sub>2</sub> to ortho-H<sub>2</sub> conversion in a full-scale automotive cryogenic pressurized hydrogen storage up to 345 bar, *International Journal of Hydrogen Energy* 39 (2014) 6533–6547. doi:10.1016/j.ijhydene.2014.01.205.
- [34] F. C. M. Sebilliau, Computational Analysis of Buoyancy Driven Flows Across Scales, Ph.D. thesis, Imperial College London, 2016.
- [35] R. A. W. M. Henkes, F. F. Van Der Vlugt, C. J. Hoogendoorn, Natural-convection flow in a square cavity calculated with low-Reynolds-number turbulence models, *International Journal of Heat and Mass Transfer* 34 (1991) 377–388. doi:10.1016/0017-9310(91)90258-G.
- [36] L. Davidson, Computation of Natural-Convection Flow in a Square Cavity, in: *Proc. Eurotherm Seminar No. 22*, Paris, 1993.
- [37] I. Release 12.0 © ANSYS, Turbulence, in: *ANSYS FLUENT 12.0 Theory Guide*, 2009.
- [38] S.-H. Peng, L. Davidson, Computation of turbulent buoyant flows in enclosures with low-Reynolds-number  $k-\omega$  models, *International Journal of Heat and Fluid Flow* 20 (1999) 172–184. doi:10.1016/S0142-727X(98)10050-4.
- [39] F. Moukalled, L. Mangani, M. Darwish, The Finite Volume Method in Computational Fluid Dynamics: An Advanced Introduction with OpenFOAM and Matlab, number 113 in *Fluid Mechanics and Its Applications*, Springer, Cham Heidelberg New York Dordrecht London, 2016. doi:10.1007/978-3-319-16874-6.

- [40] P. J. Oliveira, Raad I. Issa, AN IMPROVED PISO ALGORITHM FOR THE COMPUTATION OF BUOYANCY-DRIVEN FLOWS, *Numerical Heat Transfer, Part B: Fundamentals* 40 (2001) 473–493. doi:10.1080/104077901753306601.
- [41] S. V. Patankar, D. B. Spalding, A calculation procedure for heat, mass and momentum transfer in three-dimensional parabolic flows, *International Journal of Heat and Mass Transfer* 15 (1972) 1787–1806. doi:10.1016/0017-9310(72)90054-3.
- [42] F.-S. Lien, G. Kalitzin, Computations of transonic flow with the  $v2-f$  turbulence model, *International Journal of Heat and Fluid Flow* 22 (2001) 53–61. doi:10.1016/S0142-727X(00)00073-4.
- [43] F. Ampofo, T. G. Karayiannis, Experimental benchmark data for turbulent natural convection in an air filled square cavity, *International Journal of Heat and Mass Transfer* 46 (2003) 3551–3572. doi:10.1016/S0017-9310(03)00147-9.
- [44] E. Wang, Y. Shi, L. Zhang, J. Shi, A similar simulation of the self-pressurization process of cryogenic liquid hydrogen tank coupled with wall heat conduction, *International Journal of Hydrogen Energy* 193 (2025) 152424. doi:10.1016/j.ijhydene.2025.152424.
- [45] M. Stewart, J. P. Moder, Self-Pressurization of a Flightweight, Liquid Hydrogen Tank: Simulation and Comparison with Experiments, in: 52nd AIAA/SAE/ASSEE Joint Propulsion Conference, AIAA Propulsion and Energy Forum, American Institute of Aeronautics and Astronautics, 2016. doi:10.2514/6.2016-4674.
- [46] M. Kassemi, O. Kartuzova, Effect of interfacial turbulence and accommodation coefficient on CFD predictions of pressurization and pressure control in cryogenic storage tank, *CRYOGENICS* 74 (2016) 138–153. doi:10.1016/j.cryogenics.2015.10.018.
- [47] D. Mann, *LNG Materials and Fluids*, 1 ed., 1977.
- [48] TPSX Materials Properties Database, <https://tpsx.arc.nasa.gov/>, 2026.
- [49] N. J. Simon, E. S. Drexler, R. P. Reed, Review of Cryogenic Mechanical and Thermal Properties of Al-Li Alloys and Alloy 2219, Technical Report NIST IR 3971, National Institute of Standards and Technology, Gaithersburg, MD, 1991. doi:10.6028/NIST.IR.3971.
- [50] P. E. Phelan, M. Zhang, The Thermal Conductance of Indium-Filled Contacts at Cryogenic Temperatures, in: *Heat Transfer, Volume 2*, ASMEEDC, Anaheim, California, USA, 2004, pp. 753–758. doi:10.1115/IMECE2004-61971.
- [51] L. Salerno, P. Kittel, A. Spivak, Thermal conductance of pressed metallic contacts augmented with indium foil or Apiezon grease at liquid helium temperatures, *Cryogenics* 34 (1994) 649–654. doi:10.1016/0011-2275(94)90142-2.
- [52] S. Sunil Kumar, K. Ramamurthi, Thermal contact conductance of pressed contacts at low temperatures, *Cryogenics* 44 (2004) 727–734. doi:10.1016/j.cryogenics.2004.04.004.
- [53] K. Bellur, V. Konduru, M. Kulshrestha, D. Tyrewala, E. Medici, J. S. Allen, C. K. Choi, D. S. Hussey, D. C. Jacobson, J. B. Leão, J. McQuillen, J. Hermanson, A. Tamilarasan, Contact Angle Measurement of Liquid Hydrogen (LH2) in Stainless Steel and Aluminum Cells, *Journal of Heat Transfer* 138 (2016). doi:10.1115/1.4032232.
- [54] V. P. Carey, *Liquid-Vapor Phase-Change Phenomena: An Introduction to the Thermophysics of Vaporization and Condensation Processes in Heat Transfer Equipment*, 3 ed., CRC Press, 2020. doi:10.1201/9780429082221.