

# Numerical study of a liquid-piston compressor system for hydrogen applications

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## Abstract

The use of a liquid-piston system for hydrogen compression is investigated in this paper by means of a computational fluid dynamics (CFD) analysis. In the specific context of hydrogen-driven vehicles, high-pressure storage tanks are key to provide substantial range. The present study focuses on the intermediary compression stage of a compression-storage-dispensing (CSD) station, bringing hydrogen gas from 15 bar to 450 bar, i.e., for a pressure ratio of 30. Until now the liquid-piston technology has not been investigated for hydrogen gas compression at very high pressure, which is the purpose of this study. Simulations of the compressible two-phase flow problem are performed with a volume-of-fluid (VOF) framework using a real gas model for the gaseous phase to account for compressibility effects at large pressure ratios. A particular attention is paid to the numerical model formulation and to the treatment of the thermal boundary conditions. Results are reported using both time-resolved instantaneous bulk thermodynamic variables and global integrated quantities. Different compression scenarios are investigated, which highlights the compromise between compression efficiency and power density. To achieve the targeted pressure ratio at a power density of approximately 540 kW/m<sup>3</sup>, the compression energy cost reaches 1.67 kWh/kg. Finally the paper proposes an innovative solution to minimize cost and achieve quasi-isothermal compression, based on internal forced convection. For a similar power density, a high-speed fan in the top part of the compression chamber (modelled as a volumetric momentum source of 2500 N/m<sup>3</sup>) increases heat transfer and leads to a 25-% reduction in compression consumption.

**Keywords:** hydrogen, liquid-piston compressor, heat transfer, compressible two-phase flow, CFD

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## 1. Introduction

The transportation sector accounts for 23% of the worldwide CO<sub>2</sub> emissions according to the latest IEA report [1]. A rapid and cost-effective shift away from carbon-intensive oil-based transportation towards low-emission alternatives is key, both: (i) to meet the increasing mobility needs of people and goods; and (ii) to achieve the emission reduction targets set under the legally binding Paris Agreement international treaty, where 196 Parties agreed to reduce emissions by at least 40% by 2030 from 1990 levels. Hydrogen-powered fuel cell electric vehicles are a serious candidate to provide clean transportation and are strong competitors to lithium-ion battery electric vehicles.

Specific advantages of hydrogen-fuelled over battery electric vehicles are a longer range (for a similar weight) and significantly lower refuelling times [2], which are achieved thanks to high-pressure (up to 700 bar in recent vehicles) hydrogen tanks that can be filled quickly (typically less 5 minutes) in dedicated compression-storage-dispensing (CSD) stations. However, the main technical challenge for a rapid refuelling process is to limit the gas temperature rise due to compressive heating, while maintaining a satisfactory power density of the compressor system.

Isothermal compression is an ideal process to deliver high-pressure hydrogen at near-ambient temperature. In a typical volumetric compressor, this can be achieved for example by compressing the gas very slowly, thus leaving plenty of time for the gas to cool down during the compression process, or by reducing the compression ratio in order

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## NOMENCLATURE

|              |                       |                             |
|--------------|-----------------------|-----------------------------|
| $c_p$        | [J/kg/K]              | Specific heat capacity      |
| $C_c$        | [J/kg]                | Compression energy cost     |
| $D$          | [m]                   | Cylinder bore diameter      |
| $E$          | [J]                   | Energy                      |
| $g$          | [m/s <sup>2</sup> ]   | Gravitational constant      |
| $h$          | [W/m <sup>2</sup> /K] | Heat transfer coefficient   |
| $H$          | [m]                   | Cylinder height             |
| $m$          | [kg]                  | Mass                        |
| $M$          | [kg/mol]              | Molar mass                  |
| $n$          | [-]                   | Polytropic index            |
| Nu           | [-]                   | Nusselt number              |
| $P$          | [Pa]                  | Pressure                    |
| Pe           | [-]                   | Péclet number               |
| Pr           | [-]                   | Prandtl number              |
| $Q_v$        | [m <sup>3</sup> /s]   | Volumetric flowrate         |
| $r$          | [-]                   | Pressure ratio              |
| $t$          | [s]                   | Time                        |
| $T$          | [K]                   | Temperature                 |
| $\mathbf{u}$ | [m/s]                 | Velocity field              |
| $V$          | [m <sup>3</sup> ]     | Volume                      |
| $W$          | [J]                   | Work                        |
| $\dot{w}_c$  | [W/m <sup>3</sup> ]   | Compressor power density    |
| $x$          | [m]                   | Spatial coordinate          |
| $y^+$        | [-]                   | Dimensionless wall distance |
| $Z$          | [-]                   | Compressibility             |

### Greek letters

|           |                      |                                                     |
|-----------|----------------------|-----------------------------------------------------|
| $\alpha$  | [m <sup>2</sup> /s]  | Thermal diffusivity $\alpha = \lambda / (\rho c_p)$ |
| $\Delta$  | [m]                  | cell size                                           |
| $\gamma$  | [-]                  | Heat capacity ratio                                 |
| $\eta_c$  | [-]                  | Compression efficiency                              |
| $\lambda$ | [W/m/K]              | Thermal conductivity                                |
| $\mu$     | [kg/m/s]             | Dynamic viscosity                                   |
| $\rho$    | [kg/m <sup>3</sup> ] | Density                                             |
| $\phi$    | [W/m <sup>2</sup> ]  | Surface heat flux density                           |
| $\xi_q$   | [-]                  | $q$ -phase specific volume fraction                 |
| $\omega$  | [rad/s]              | piston angular frequency                            |

### Subscripts

|       |                                 |
|-------|---------------------------------|
| 0     | Initial condition (at $t = 0$ ) |
| c     | Compression                     |
| crit  | Critical state                  |
| end   | End of the compression stroke   |
| g     | Gas phase                       |
| i     | Inner-wall boundary             |
| iso   | Isothermal                      |
| l     | Liquid phase                    |
| o     | Outer-wall boundary             |
| $q$   | Phase indicator                 |
| s     | Solid phase                     |
| w     | Wall                            |
| $\Re$ | Real part                       |
| $\Im$ | Imaginary part                  |

### Acronyms

|      |                                 |
|------|---------------------------------|
| CAES | Compressed air energy storage   |
| CFD  | Computational fluid dynamics    |
| CSD  | Compression-storage-dispensing  |
| EOS  | Equation of state               |
| IEA  | International Energy Agency     |
| PCM  | Phase change material           |
| RANS | Reynolds-averaged Navier Stokes |
| VOF  | Volume of fluid                 |

to maximise the cooling heat flowrate. However, in both cases, this is done to the detriment of the power density. A good compromise between efficiency and power density is thus to be found. Previous works have focused on optimising the compression/expansion trajectories in this context [3–5]. Optimisation generally leads to segments of fast compression at the beginning, where cooling of the compressed gas is not primordial, and slow compression near the end of the process to maximise this cooling, which generally relies on the use of liquid pistons, the motion of which is easily controlled through adjusting the feeding pump speed. The current study however focuses on fixed-flowrate liquid-piston compressors, the target being to reduce the energy cost for a given power density. Given the power-law growth of pressure during compression, it is important to keep in mind that using a fixed water flow rate requires adequate sizing of the pump engine or a combination with inertia disk.

Reciprocating-piston devices present specific advantages over competing volumetric compression/expansion machines (e.g., screw or scroll technologies), including large built-in volume ratios and ability to operate with two-phase working fluids (e.g., liquid spray cooling or wet compression). Piston machines have thus been proposed for use in waste-heat recovery applications [6], combined heat and power systems using organic Rankine cycle (ORC) engines [7], and pumped thermal electricity storage technologies (also known as Carnot batteries) [8]. In this study, a liquid-piston system is considered to compress hydrogen. Liquid-piston compressors allow to replace the mechanical transmission via a crankshaft system by a hydraulic pump, thus reducing the number of moving parts and removing the need for piston rings to prevent mass leakage. Liquid-piston systems provide even further advantages in comparison to standard reciprocating-piston devices [9], including perfect sealing property, cooling effect from the liquid and more particularly suitability of use in combination with heat transfer enhancers. A thermal analysis of a liquid piston compressor was performed by Patil et al. [10] but it concerned small pressure ratios below 2.5.

Near-isothermal compression can be achieved by maximising heat removal from the compressed gas. In the last decade, several systems have been developed and designed to increase heat transfer within liquid-piston compressors. As stated previously, adjusting the speed of the liquid piston is one of the possibilities [11]. Another possibility is the use of walls with embedded phase change materials (PCMs), as proposed by Mazzucco et al. [12]. In this case, part of the compression heat is absorbed as latent heat by the PCM at constant temperature. The effect of moisture on the compressor performance was also investigated by Srivatsa and Li [13]. Another approach is to increase the heat transfer surface area between the gas, and either the liquid or additional inserted solids. Heat transfer enhancement based on large surface area and heat transfer coefficient of aqueous foam has been experimentally studied by Patil & Ro [14]. Liquid droplets spraying is another solution regarding the former approach and has been investigated for both standard reciprocating compressor devices [15] and liquid-piston compressors [16–18]. The energy cost required to generate the liquid drops at high pressure can be mitigated by pumping the already-pressurised water from the bottom of the piston. This is then performed with an additional high pressure pump at an additional financial cost. Finally, for the latter method, the use of porous metal inserts of high thermal inertia [19, 20] also allows maximisation of the heat transfer by increasing the gas-to-solid surface area. To the authors' knowledge, the only experimental study of this concept at high pressure ratio is presented by Wieberdink et al. [20]. Numerically, the combination of a liquid-piston system and porous metal foam has been studied in Refs. [21–23] for compressed air energy storage (CAES) applications. Zhang et al. [24] developed CFD models to investigate the design of an empty compression chamber to optimise compression.

Hydrogen tank filling has been widely studied with CFD in literature in single-phase flow configurations [25–30], with studies focusing mainly on the thermal distribution within the reservoirs, the local peaks of temperature and the heat transfer across solid walls. However, the use of liquid-piston systems for the compression of hydrogen gas is scarce. This can be due to the limitations inherent to such systems, such as potential mass transfer between both phases. For this reason, the study of Wang et al. [31] is based on an ionic liquid compressor playing the role of the piston. Ionic liquids have no vapour pressure, allow for low gas solubility and have a high corrosion resistance. In case mass transfer is not avoided during compression, separator technologies can be used to recover the materials purity, but at additional cost. Kermani and Rokni [32] proposed a 0D/1D thermodynamic model to predict hydrogen compression with a liquid-piston system. Their results show that water-hydrogen interface does not play an important role in cooling the gas during compression. The study is however limited to a pressure ratio of 5 and only account for conduction at the interface. The results discussed in the present paper show on the contrary an important contribution from the interface for the considered configuration with high pressure ratio. The present study proposes remedying the existing research gap concerning the evaluation of the potential of the liquid-piston concept in terms of cost and efficiency for hydrogen gas compression at very high pressure. The first innovative contribution of this paper is related

to the critical question regarding the reduction of the compression energy cost in high-pressure compressor devices. A detailed literature survey has been provided above on the different ways to achieve quasi-isothermal compression. In this paper, we present a new method for running the compression stage with a reduced energy cost. The solution is based on the use of an internal fan that generates a convection loop within the compression space, thus enhancing gas-to-wall and gas-to-liquid heat transfer and effectively cooling down the gas during compression. The potential of this method in terms of reduction of the compression consumption is assessed quantitatively and the results are promising as the compression efficiency increases from 71% to 95% for the cases considered. The second innovative contribution is the proposition of a complex Nusselt-Peclet correlation describing the gas-to-wall heat transfer during the compression stroke, which exhibits strong transient effects. This correlation accounts for the unsteady behaviour of the gas-to-wall heat transfer, which is well observed with our numerical results, and thus described in the manuscript. The underlying physics is highlighted in Section 2.2.

One of the inherent difficulties associated with hydrogen compression for the transportation sector lies in the transient nature of the thermodynamic process. Unlike reciprocating devices, the totality of the compressed gas is ideally discharged at the end of the compression phase in liquid-piston systems. The whole process thus includes a full-stroke admission, a compression and an exhaust phase. The compression phase being the most expensive phase, the present study is aiming at estimating and minimizing its associated energy consumption.

The liquid-piston system is described in Section 2. The physical and numerical modelling are then discussed in Section 2. A particular attention is paid to the relevance of the wall thermal boundary condition and to the computation of the wall heat transfer. Results are presented in terms of energy cost for different water flow rate, pressure ratio and initial pressure level. Finally, Section 4.3 shows that significant cost reduction can be obtained by imposing a forced convective loop.

## 2. Liquid-piston compressor

### 2.1. Working principle

The working principle of a liquid-piston compressor is to vary the gas volume by pumping a hydraulic fluid within the compression chamber at a controlled flowrate,  $Q_v$ . The liquid-piston is designed for a vertical arrangement, and a schematic of the system is shown Figure 1. The compression chamber is cylindrical (with length  $L$  and diameter  $D$ ). In comparison with reciprocating-piston devices, the mechanical transmission via a crankshaft system is replaced by a hydraulic pump, thus reducing the number of moving parts and removing the need for piston rings to prevent mass leakage. In a simple configuration without inserts in the cylinder, the gas exchanges heat with the surroundings via conjugate convective-conductive heat transfer through the cylinder walls and with the liquid piston via convection at the gas-liquid interface.

The two key quantities to determinate the cost effectiveness of the present compressor system, and thus its potential industrialisation, are the cost of compression of a certain amount of hydrogen and the power density of the required

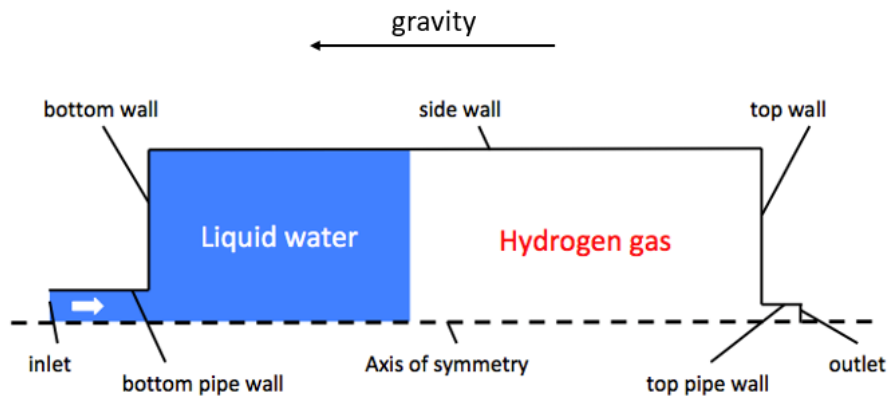


Figure 1: Schematic diagram of the liquid-piston compressor system.

compression. The compression energy cost,  $C_c$ , is evaluated by integrating the input work,  $W_c$ , during compression and includes as well the discharge stage of the compressed gas at the end. This cost reads:

$$C_c = \frac{W_c}{m} = -\frac{1}{m} \int_{V_0}^{V_c} (P - P_0) dV + (rP_0 - P_0)V_c, \quad (1)$$

where  $r$  and  $m$  stand respectively for the pressure ratio and the mass of hydrogen gas. The integration is performed between the initial gas volume,  $V_0$ , and the volume of gas at the end of the compression,  $V_c$ . End of compression is fixed as the time when  $r = 30$  for all computations. The discharge step is supposed to happen at constant pressure and the dead volume at the end of the process is assumed to be null for sake of simplification. The input work is minimal when the compression is isothermal. The compression efficiency is thus defined as the ratio between the work of an isothermal compression,  $W_{iso}$ , in similar configurations, and the current input work:

$$\eta_c = \frac{W_{iso}}{W_c}, \quad (2)$$

The isothermal compression work can be obtained from the isothermal evolution of hydrogen modeled for instance by the CoolProp library [33], which accounts for real gas behaviour. Another option is to calculate the reversible isothermal compression work using the specific gas entropy  $s$  as following:

$$W_{iso} = T_0 m (s_c - s_0) + P_0 (V_c - V_0) + V_c (rP_0 - P_0). \quad (3)$$

Finally, the power density,  $\dot{w}_c$ , is defined as the ratio of the isothermal compression power (i.e., the ratio of the isothermal work to the compression time,  $t_c$ ) to the reference volume:

$$\dot{w}_c = \frac{W_{iso}}{t_c V_0}. \quad (4)$$

## 2.2. Unsteady gas-to-wall heat transfer for standard reciprocating device

The diabatic compression of a gas is polytropic by nature, which explains the power-law evolution of the temperature as function of the volume: a polytropic process obeys the well-known  $TV^{n-1} = C$  relationship, where  $C$  is a constant and  $n$  the polytropic index (or exponent), which equals 1 for an isothermal process and  $\gamma$  for an adiabatic process. On the one hand, the lower the liquid-piston velocity, the more time is available for gas-to-wall heat transfer (which in turn allows the gas to reach near thermal equilibrium with the solid walls), the closer to isothermal is the compression process ( $n \rightarrow 1$ ). On the other hand, for high piston-piston velocity, little time is left for the heat transfer to significantly relax the temperature profile in the gas phase, and the compression approaches an adiabatic process ( $n \rightarrow \gamma$ ).

As for the gas-to-wall heat transfer coefficient, a highly-transient observation has been observed in previous theoretical [34, 35], experimental [36, 37] and numerical [37, 38] investigations and can be explained qualitatively. Unsteady pressure-driven heat transfer in reciprocating-piston devices has attracted significant interest in the past decades. In the early 40s, Pfriem [34] predicted a phase shift between the instantaneous gas-wall temperature difference and the gas-to-wall heat flux, thus leading to infinite values of the heat transfer coefficient as defined in the Newton's law of cooling. Similar results were predicted by an analytical description of the gas thermal boundary layer proposed by Lee in 1983 and has been evidenced experimentally by various experimental investigations, e.g. that by Kornhauser and Smith [36]. From a phenomenological perspective, this singularity is now well understood in reciprocating-piston gas spring [37, 39]. The singularity is the result of heat accumulation in the boundary layer in the early phase of compression: in the wall vicinity the gas temperature is higher than the wall temperature, while the bulk gas temperature is still colder than the latter (see Figure 2).

Let us now consider the very system studied in this paper. Initially, the hydrogen within the compression chamber is at homogeneous temperature and in thermal equilibrium with the surrounding stainless steel walls. Once the compression starts, compressive heating is acting as a volumetric heat source, which heats up the whole gas including that closest to the wall. An infinitesimally small time later, the gas temperature has risen homogeneously, while the wall temperature remained constant. Using the Newton's law of cooling thus leads to predicting an infinite value of the

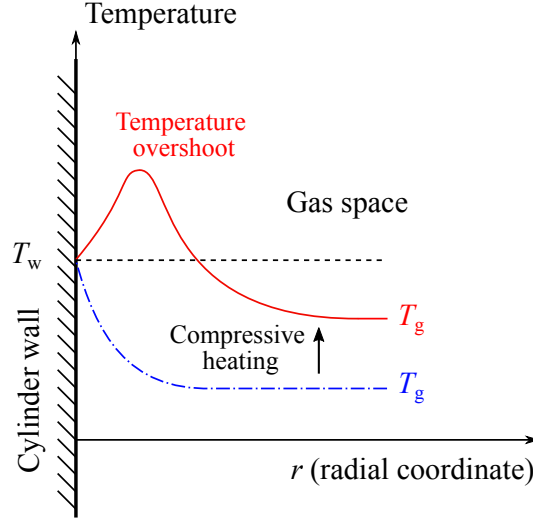


Figure 2: Schematic representation of the change in the in-cylinder gas temperature profile during the compression stroke.

heat transfer coefficient. As the piston keeps moving upwards, time is allowed for the temperature profile to relax via heat diffusion, thus leading to decreasing, finite Newton-coefficient values.

The initial value of the gas-to-wall convective heat-transfer coefficient (as defined in the Newton's law of cooling) approaching infinity in the current study and the phase shift observed between the instantaneous gas-wall temperature difference and heat flux are both due to the thermal inertia of the compressible gas thermal boundary layer. To account for the latter, Kornhauser and Smith [36] proposed in 1994 a novel expression for the instantaneous convective heat flux,  $\phi_w$ , by using a complex Nusselt number,  $Nu_c = Nu_{\Re} + iNu_{\Im}$ :

$$\phi_w = \frac{\lambda_{g,w}}{D_h} \left[ Nu_{\Re} (\langle T_g \rangle - T_w) + \frac{Nu_{\Im}}{\omega} \frac{d\langle T_g \rangle}{dt} \right], \quad (5)$$

where  $\langle T_g \rangle$  denotes the mass-averaged gas temperature,  $k_{g,w}$  the gas thermal conductivity at the wall (i.e., at the gas mean pressure and wall temperature,  $T_w$ ),  $D_h$  the hydraulic diameter, and  $\omega$  the piston angular frequency. For the non-periodic unsteady compression process investigated in this study, we propose calculating the latter as  $\omega = \pi/\tau$ , with  $\tau$  being the compression stroke duration. Kornhauser and Smith [36] derived an empirical correlation for both real and complex parts of the Nusselt number as a function of the oscillatory Péclet number,  $Pe_\omega$ :  $Nu_{\Re} = Nu_{\Im} = 0.56 Pe_\omega^{0.69}$ . This correlation, although well suited for low compression ratios, is not adapted for the large pressure ratios investigated in our study. For the latter cases, Lekić proposed an improved formulation in his PhD dissertation [40]:

$$Nu_{\Re} = a_{\Re} + b_{\Re} Pe_\omega^{c_{\Re}}, \quad \text{and} \quad (6)$$

$$Nu_{\Im} = a_{\Im} + b_{\Im} Pe_\omega^{c_{\Im}}, \quad (7)$$

where the Péclet number,  $Pe_\omega$ , is defined as:

$$Pe_\omega = \frac{\omega D_h^2}{4 \bar{\alpha}}, \quad (8)$$

with  $\bar{\alpha}$  being the time- and mass-averaged gas thermal diffusivity.

### 2.3. Forced internal convection for the new device

The possibility of maximising the convective heat transfer between the gas and both liquid and solid surfaces during the compression process is lastly investigated. As any convective heat transfer is of the form  $Q = hA\Delta T$ , an increase in heat transfer rate can be achieved either by maximising the heat transfer area,  $A$ , or by maximising the heat transfer coefficient,  $h$ . This second option is studied in this paper. Enhancing internal convection is achieved by

artificially forcing a downward motion of the gas, which is representing the effect of an axial pump or fan. We thus investigate the idea of using an axial fan inside the chamber, at its top extremity. As the water is slowly going up, the fan will push the hot gas downward and will increase velocities at the interfaces with the liquid and the solid wall. At the very end of the compression stroke and during the exhaust phase, the fan will be submerged by water, which will ultimately stop its rotating motion. There are several options to design such a system, for which the two most relevant are shortly discussed. The first method is to drive the fan with a shaft connected to a turbine located at the bottom of the reservoir. The turbine will be itself driven by the ascending pumped water. The drawback of this method is that the fan speed, and thus its cooling potential, is directly dependent on the water flow rate within the tank. The second option is to use an independent waterproof brushless DC motor to drive the rotating fan. However, specific care must be taken regarding its resistance to high pressure and temperature, as well as potential leaking where the motor connection cables exits the tank.

### 3. Modelling

The different physical and numerical models considered to predict the operation of the liquid-piston compressor are firstly introduced in this section. Secondly, the validation of the model is presented.

#### 3.1. Governing equations

Due to the high compression experienced by the gas, the compressible viscous Navier-Stokes equations are considered in the present study. An equation of state (EOS) is used for the gas for the thermodynamic closure of the governing equations. The compressibility of liquid water is neglected. Given its high bulk modulus, this leads to a maximum error below 2% for the liquid volume at 450 bar. A volume-of-fluid (VOF) approach is used to deal with the two-phase nature of the system. The choice of the VOF formulation has been driven by the high pressure ratio investigated in this study. Single-phase flow approaches with moving and adaptive meshing, such as those performed by Lekic and Kok [38] or Willich et al. [41], are limited to low pressure ratios due to the strong distortion of the mesh. Cell merging techniques can be used to address this issue but are computationally expensive. The liquid-to-gas mass transfer is neglected. Water evaporation has not been clearly quantified to the authors' knowledge for this type of system. Wieberdink et al. [20] did not mention this issue during the operation of their liquid-piston system for air compression at very high pressure. We assume that the thermal stratification, which is visible in the presentation of the results in Section 4.1, leads to a gas temperature in the vicinity of the interface low enough to limit evaporation. The set of governing equations finally reads:

$$\left\{ \begin{array}{l} \frac{1}{\rho_g} \left[ \frac{\partial}{\partial t} (\xi_g \rho_g) + \nabla \cdot (\xi_g \rho_g \mathbf{u}) \right] = 0 \\ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \\ \frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla P + \nabla \cdot [\mu (\nabla \mathbf{u} + \nabla^T \mathbf{u})] + \rho \mathbf{g} \\ \frac{\partial}{\partial t} (\rho E) + \nabla \cdot (\mathbf{u} (\rho E + P)) = \nabla \cdot (\lambda \nabla T) \end{array} \right. \quad \begin{array}{l} (9a) \\ (9b) \\ (9c) \\ (9d) \end{array}$$

The continuity equation is solved for the gas-phase volume fraction,  $\xi_g$ , while the volume fraction of the liquid phase is obtained from the mass balance  $\sum_q \xi_q = 1$ , with  $q = (g, l)$  the phase indicator. Single momentum and energy equations are solved throughout the domain, and the resulting velocity  $\mathbf{u}$  is shared among the phases, while the density  $\rho$  and the viscosity  $\mu$  are phase-dependent. The energy,  $E$ , and temperature,  $T$ , are treated as mass-averaged variables in each grid cell.

Due to the much higher thermal inertia of water compared to hydrogen, the maximum interface temperature only reaches 54 °C at the very end of the compression for the worst case scenario. Therefore the liquid density is assumed temperature independent, as for its other properties. For the gas phase, the buoyancy effect is directly taken into account through the EOS. Given the high pressure achieved in this study, the ideal gas law is not suitable to capture the variation of equilibrium properties throughout the compression stroke. The Peng-Robinson EOS [42] is therefore used for the present study. Regarding the thermal conductivity,  $\lambda$ , the kinetic theory based on Eucken relation is

employed for hydrogen. For liquid water, the thermal conductivity is computed based on the Prandtl number,  $Pr$ . The variations of the hydrogen heat capacity,  $c_p$ , and viscosity,  $\mu$ , with temperature are respectively based on a 5<sup>th</sup>-order polynomial function [43] and Sutherland's law.

### 3.2. Presentation of the numerical model

CFD computations are performed with ANSYS Fluent v15. The QUICK (quadratic upstream interpolation for convective kinematics) scheme is used to discretise the volume fraction equation, while a second-order upwind scheme is used for the spatial discretisation of other variables. A first order implicit scheme is used for the time discretisation, with the time step determined from a convergence study to ensure independence of the results upon the time step size. Finally, a RANS approach based on the  $k-\omega$  turbulence model with low-Reynolds corrections is used for turbulence modelling.

Given the simple geometry of the compressor system, and the fact that the gravity vector is parallel to the tank axis of symmetry, an axi-symmetric computational domain is considered. This allows a significant reduction of the computational cost. In order to study the physics of the compression and expansion processes, a simplified computational domain without inlet and outlet pipes is considered. With such simplified domain, the water entrance jet at the bottom of the tank is not predicted, and the gas-liquid interface remains horizontal during compression/expansion. In reality this water jet is responsible for the interface curvature, at the start of the compression. The curvature's level depends on the water flow rate. A maximum disturbance height of  $0.08H$  and  $0.002H$  have been respectively obtained for the highest and lowest flow rates, considering a pipe inlet diameter of  $0.15D$  and an initial water level of  $0.3L$ . The induced mixing eventually enhances slightly the heat transfer. The interface remains however fairly stable at the end of the compression, where most of the compression work is to be achieved. Both thermal and momentum influences of the water jet can be reduced if needed by increasing the initial level of water in the tank or by increasing the inlet pipe diameter.

The ascending water flow inside the chamber is obtained by imposing a constant positive and uniform velocity at the inlet boundary. Its magnitude is adjusted to satisfy the desired water flow rate and compression time. Except for the inlet boundary, all other boundaries represent closed surfaces during the whole compression. They are therefore modeled as no-slip wall, with a zero pressure gradient condition. The walls thermal boundary condition is discussed in the next Section. Initially, the static pressure is set to 15 bar and a pressure ratio of 30 is aimed at. The initial temperature is set to 20 °C, and the tank is initially filled with water up to  $0.3H$ . The mesh is made of rectangular cells of perfect orthogonal quality. Inflation layers are included at all wall boundaries.

### 3.3. Validation of the numerical model

The numerical accuracy of the present model is supported by (i) a grid independence study and (ii) a comparison to experimental tests [20], which are both discussed in this section.

A grid convergence study is performed to ensure reproducibility of the numerical results. Three levels of refinement are considered in this study for the computational grid. The characteristics of the three grids are listed in Table 1. These simulations were performed with a flow rate of 3 L/s. Walls are considered isothermal, which corresponds to the limit case of maximum wall heat transfer. As seen with the values of the dimensionless wall distance,  $y^+$ , the first wall cell layer for both medium and fine grids lies within the laminar viscous part of the momentum boundary layer. As for the thermal boundary layer, results are discussed below.

Table 1: Numerical parameters and results of the grid convergence study. Results reported here are taken from simulations performed for a constant water inlet flowrate of 3 L/s, with isothermal walls at 20 °C and starting from a static pressure of 15 bar .

| Mesh            | Cell count | Normalized min. cell size $\frac{\Delta}{D}$ [-] | $y_{mean}^+$ | $y_{max}^+$ |
|-----------------|------------|--------------------------------------------------|--------------|-------------|
| Grid 1 (coarse) | 2400       | 0.25%                                            | 4.8          | 9.2         |
| Grid 2 (medium) | 8400       | 0.062%                                           | 2.2          | 4.9         |
| Grid 3 (fine)   | 29600      | 0.0016%                                          | 1.0          | 2.5         |

Regarding the evolution of the pressure during the compression process, a good agreement is already found between the results of the medium and the fine grid. As for the bulk gas temperature, the evolution is shown in Figure 3a.

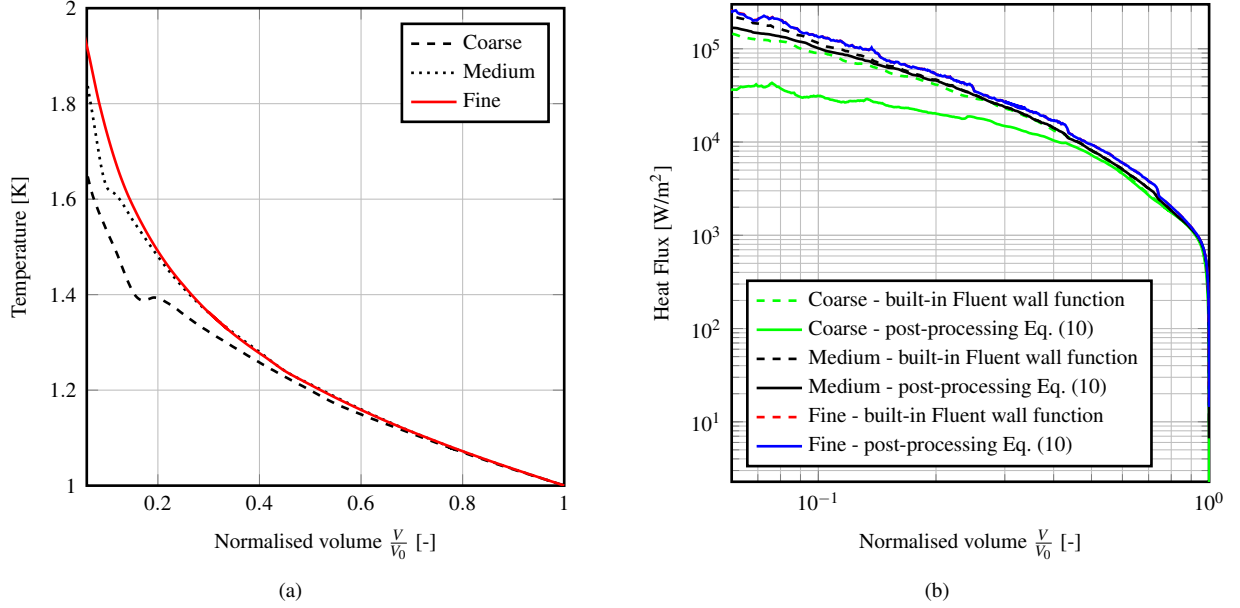


Figure 3: Time-resolved evolution of thermodynamic parameters as functions of the normalised gas volume for three different computational grid density: (a) normalised volume-averaged hydrogen temperature; and (b) surface-averaged gas-to-wall heat flux at the side wall measured: (i) using the built-in Fluent wall functions; and (ii) in post-processing from the computed temperature fields according to Eq. (10). Results reported here are taken from simulations performed for a constant water inlet flowrate of 3 L/s, with isothermal walls at 20 °C and starting from a static pressure of 15 bar. Further details on the coarse, medium and fine grids are provided in Table 1.

It appears that the coarser grids predict lower gas temperatures and fail at predicting the gas temperature evolution with satisfying accuracy, as shown by the large discrepancies observed between the temperature-volume trace with coarse medium grids and that obtained with a fine grid. In addition, the temperature obtained with the fine grid follows a near-polytropic evolution during the whole compression process, as already observed experimentally in Ref. [19, 20]. Although the polytropic index is not necessarily constant throughout the process, polytropic models are often used to predict the performance of reciprocating-piston devices [40] (except near bottom and top dead centers), and that of liquid-piston compressors at constant flow rates [19, 20]. Interestingly, Yan et al. [19] have observed that expansion processes with non-constant flow rates do not fit polytropic models. These results suggest that Grid 3 is sufficiently fine for the present problem. This conclusion is supported by the heat flux evolution at the walls. Figure 3b presents the surface averaged heat flux for the gas phase at the side wall in contact with the gas, for the medium and the fine grids. The heat flux is computed using ANSYS Fluent formulation based on temperature wall functions [44], and compared to the laminar heat flux measured in post-processing from the computed temperature field:

$$\phi_w = -\lambda_g \frac{\partial T_g}{\partial x} \Big|_w, \quad (10)$$

where  $\phi_w$  represents the gas-to-wall surface heat flux density,  $\lambda_g$  is the local gas thermal conductivity and  $x$  represents the spatial coordinate normal to the wall. With the coarse grid, the difference between the two ways of computing the heat flux is significant. With the medium grid, a non-negligible difference is also found for a volumetric ratio above 5. On the contrary, the thermal boundary layer is sufficiently resolved with the fine grid for the two heat flux calculations to coincide perfectly. One can note that the correlation from Fluent gives a satisfactory prediction of the real heat flux even with coarse grids. Given the Prandtl number close to unity, one can expect having thermal boundary layer thickness close to the viscous boundary layer thickness (see Table 1). The gas velocity within the latter layer exhibits small fluctuations during the thermodynamic evolution, which are leading to little step changes of the heat flux visible in Figure 3b.

The accuracy of the numerical model presented above is finally verified by comparison with experimental measurements performed by Wieberdink et al. [20]. Like our system, the experimental tests deal with a high pressure liquid-piston compressor. Two baseline scenarios are reproduced numerically for two different piston speeds: (i) 800cc/s which corresponds to a 2.7s compression stroke and (ii) 100cc/s which corresponds to a 22s compression stroke. The compressed gas is air which is modelled as a real gas with Peng-Robinson equation of state. Air is compressed from 7 to 210 bar, and is initially at 310 K. Isothermal wall conditions are considered for the comparison, similarly to the present investigation. Figure 4 shows the evolution of the pressure ratio and the normalised temperature obtained numerically, along with the experimental data. A very good agreement is found between numerical and experimental measurements, for both piston speeds. It is worth keeping in mind that compensating discrepancies may coexist, as the isothermal wall boundary condition may overestimate the gas-to-wall heat transfer and thus the resulting gas cooling effect, while the evaporation process which is not taken into account in the numerical model may on the contrary underestimate the cooling effect. However, the latter issue has not been mentioned in [20]. In addition, stainless steel walls are used by the authors, which allows the limitation of the increase of the inner-wall surface temperature.

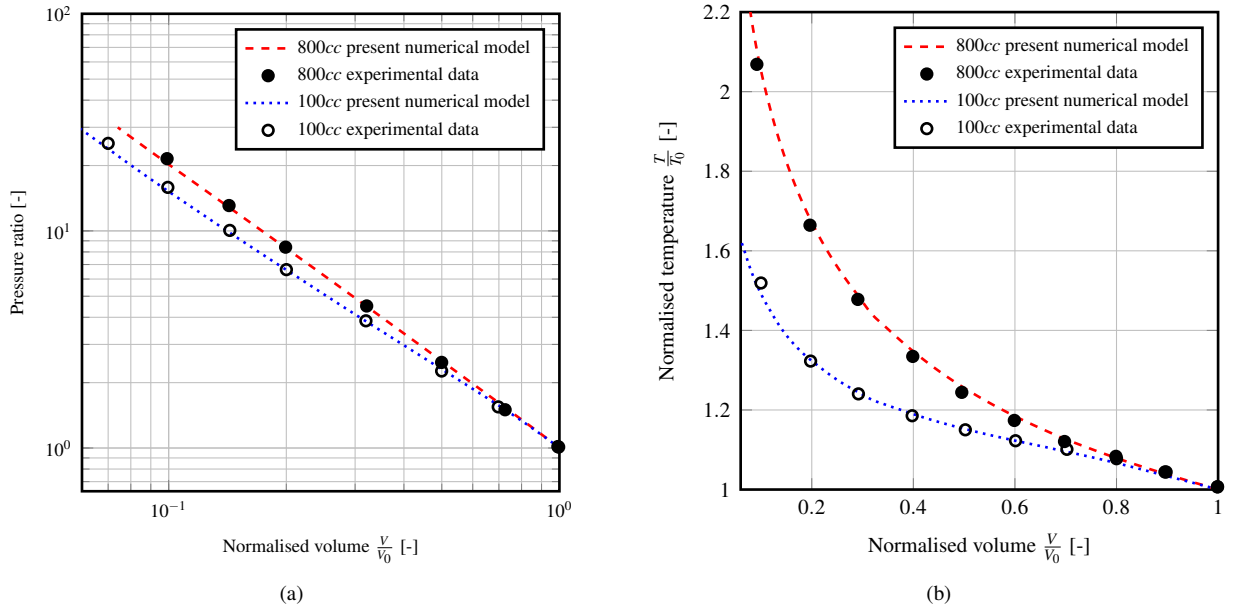


Figure 4: Time-resolved evolution of thermodynamic bulk parameters as functions of the normalised gas volume along the experimental data from [20] for two piston speeds: (a) pressure evolution; and (b) temperature evolution

## 4. Results and discussion

The gas-to-wall heat transfer during the compression stroke is firstly analysed in Section 4.1. The co-influence of injection flowrate, initial pressure, pressure ratio and wall thermal boundary conditions on the compression energy cost and efficiency is then explored in Section 4.2. Finally, the potential of forced internal convection using fans within the compression chamber to reduce the overall pumping work is investigated in Section 4.3. Baseline initial, operating and boundary conditions of the liquid-piston compression system are detailed in Table 2.

### 4.1. Unsteady gas-to-wall heat transfer and in-cylinder wall temperature variations

The unsteady gas-to-wall heat transfer is analysed in this Section. The inner-wall thermal boundary condition allows maximisation of the gas-to-wall heat transfer and thus reduction of the compression energy cost. The requirements for keeping this condition are then discussed within this section through a one-dimensional analysis of the gas-to-wall thermal boundary layer.

Table 2: Baseline initial, operating and thermal boundary conditions.

| Initial conditions                 |                                   |
|------------------------------------|-----------------------------------|
| Initial hydrogen pressure          | $P_0 = 15 \text{ bar}$            |
| Initial hydrogen temperature       | $T_0 = 20 \text{ }^\circ\text{C}$ |
| Initial compression chamber volume | $V_0 = 31.72 \text{ L}$           |
| Operating conditions               |                                   |
| Overall pressure ratio             | $r = 30$                          |
| Injection flowrate                 | $Q_v = 3 \text{ L/s}$             |
| Thermal boundary conditions        |                                   |
| Isothermal inner-wall temperature  | $T_w = 20 \text{ }^\circ\text{C}$ |

Time-resolved evolutions of the inner heat transfer coefficient,  $h_i$ , and bulk gas temperature,  $T_g$ , governed by the volumetric compression rate, are shown for two extreme liquid-piston speeds (reported using inlet water flow rates  $Q_v = 3 \text{ L/s}$  and  $Q_v = 0.3 \text{ L/s}$ ) in Figure 5(b) and 5(a), respectively. The bulk gas temperature is accurately captured by a power-law regression. For the high piston velocity, a polytropic index of approximately 1.2 is obtained. A lower value of 1.05 is found for the lower piston speed, which allows more time for gas-to-wall heat transfer. The highly-transient evolution of the heat transfer coefficient is verified in Figure 5, with extremely high value in the early phase of the compression, as explained in Section 2.2.

All six heuristic parameters used in Eqs. (6) and (7) involved in the complex Nusselt-Peclet correlation have been determined numerically from the processed CFD simulation data. The resulting heat transfer coefficients are reported along with the values measured from the simulations in Figure 5(b), for both the rapid ( $Q_v = 3 \text{ L/s}$ ) and slow ( $Q_v = 0.3 \text{ L/s}$ ) compression processes. The use of a complex Nusselt number, accounting for heat accumulation within the thermal boundary layer, proves well suited for such unsteady heat transfer mechanisms as the initial singularity is well captured. This can be useful for instance to create lumped models of similar systems.

Given the relatively high thermal diffusivity of stainless steel, one can expect small variations in the temperature of the inner-wall surface in contact with the compressed gas. This however depends strongly on the dynamics of the compression process. The heat diffusion through the stainless-steel walls is thus investigated thanks to a transient one-dimensional (1D) heat-conduction analysis along the thickness of the wall, in order to: (i) quantify the amplitude of the inner wall-surface temperature; (ii) determine whether a constant (isothermal) inner-wall temperature assumption is justified for the full three-dimensional transient CFD problem; and if not (iii) determine the wall material characteristics required to approach as most as possible such condition.

The unsteady heat diffusion equation is firstly solved within a finite-thickness 1D stainless steel slab subject to two Newton boundary conditions at its outer surfaces, for which the set of governing equations reads:

$$\begin{cases} \rho_s c_{p,s} \frac{\partial T_s}{\partial t} = \lambda_s \frac{\partial^2 T_s}{\partial x^2}; \\ -\lambda_s \frac{\partial T_s}{\partial x}|_o = h_o (T_{\text{amb}} - T_{s,o}); \\ -\lambda_s \frac{\partial T_s}{\partial x}|_i = h_i (T_{s,i} - T_g). \end{cases} \quad (11)$$

In Equation (11),  $T_s(x, t)$  is the solid-wall temperature profile;  $\rho_s$ ,  $c_{p,s}$  and  $\lambda_s$  are the density, specific heat capacity and thermal conductivity of stainless steel, respectively.  $T_{s,i}$  and  $h_i$  denote the in-cylinder wall temperature and gas-to-wall heat transfer coefficient, while  $T_{s,o}$  and  $h_o$  are the outer wall temperature and wall-to-ambient air heat transfer coefficient, respectively. Typical heat transfer coefficient  $h_o = 10 \text{ W/m}^2\text{K}$  [25, 26, 45] and ambient temperature  $T_{\text{amb}} = 20 \text{ }^\circ\text{C}$  are considered for the heat transfer at the air-facing outer surface of the wall. For the inner (i.e., hydrogen-facing) wall surface, the heat transfer properties (gas temperature and heat transfer coefficient) are taken from the processed CFD simulation data (presented in Figure 5), obtained with an isothermal wall boundary condition. An implicit finite-difference method is used to solve Eq. (11) numerically and obtain spatially- and time-resolved

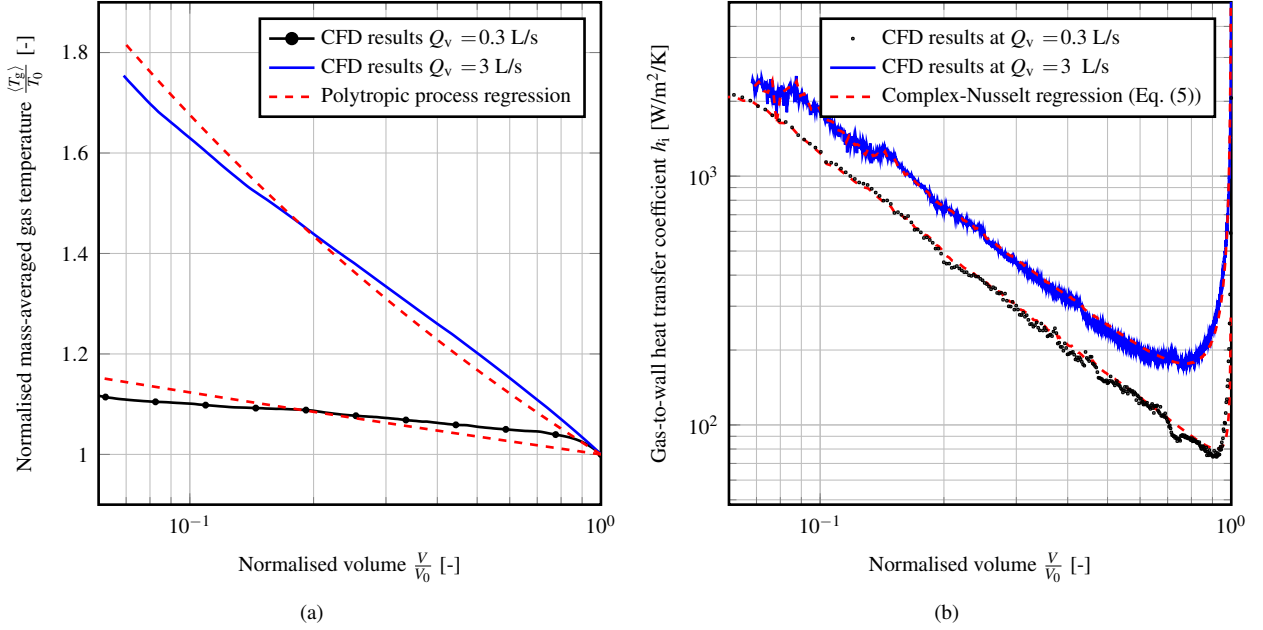


Figure 5: CFD time-resolved results and non-linear regressions for both rapid ( $Q_v = 3$  L/s) and slow ( $Q_v = 0.3$  L/s) compression processes starting from a static pressure of 15 bar with isothermal walls at 20 °C: (a) mass-averaged gas temperature reported against the normalised volume ( $V/V_0$ ) together with power-law regressions corresponding to ideal polytropic processes –  $\langle T_g \rangle = T_0(V/V_0)^{1-n}$ , with  $n = 1.05$  and  $n = 1.22$  for the 0.3-L/s and 3-L/s cases, respectively; and (b) overall gas-to-wall heat transfer coefficient reported against the normalised compression chamber volume together with interpolated complex-Nusselt correlations – see Eqs. (5-7) with  $a_{\mathfrak{K}} = -1.2 \times 10^4$ ,  $b_{\mathfrak{K}} = 1.4 \times 10^4$ ,  $c_{\mathfrak{K}} = -2.4 \times 10^{-2}$ ,  $a_{\mathfrak{G}} = -4.9 \times 10^3$ ,  $b_{\mathfrak{G}} = 4.8 \times 10^3$ ,  $c_{\mathfrak{G}} = 5.3 \times 10^{-3}$  for the 0.3-L/s case, and  $a_{\mathfrak{K}} = -2.6 \times 10^3$ ,  $b_{\mathfrak{K}} = 1.1 \times 10^4$ ,  $c_{\mathfrak{K}} = -0.22$ ,  $a_{\mathfrak{G}} = -666$ ,  $b_{\mathfrak{G}} = 13.8$ ,  $c_{\mathfrak{G}} = 0.63$  for the 3-L/s case.

temperature profiles in the solid walls. The results of this investigation are reported in Figure 6 for both rapid and slow compression processes ( $Q_v = 3$  L/s, and  $Q_v = 0.3$  L/s, respectively).

Variations in inner-wall surface temperature are significantly lower than bulk gas temperature variation in both rapid and slow compression processes. At the end of the compression stroke, the in-cylinder wall temperature reaches 50 °C (i.e., a 30-°C increase) for a large inlet water flowrate, as observed in Figure 6a, while only rises up to 32 °C (i.e., a 12-°C increase) for a low flowrate, as observed in Figure 6b. However, when compared to the temperature lift in bulk hydrogen temperature – which equals 260 °C and 38 °C in the rapid and slow processes, respectively, it appears that the inner-wall temperature variation is more significant in the slow compression process, for which the in-cylinder wall temperature increase represents 30% of the gas temperature lift. In other words, while the isothermal-wall assumption is well justified for rapid compression cases, non-negligible conductive-convective heat transfer conjugation effects occur for slow processes as more time is allowed for heat accumulation within the walls. In the latter case, the temperature gradient across the walls is significantly smaller, with a maximum of 5 °C temperature difference between the inner-wall and outer-wall temperatures. It is also worth noting that the present analysis considers a single compression step and does not account for heat accumulation within walls for consecutive compression cycles.

In order to better sustain the isothermal condition, which allows a maximum gas-to-wall heat transfer, different types of wall are secondly investigated. In addition to the stainless steel firstly considered (AISI 410), two additional materials are also investigated, namely a low carbon tool steel (AISI P3) and an Aluminium 7000 series (AL 7068). The readers can refer to Ref. [46] for the material properties. Two wall thicknesses, noted as  $\epsilon$  are also used, where the thinnest follows recent ISO standard 9809-1:2019 for high pressure gas cylinder [47] for the given diameter. Biot number values, based on the wall thickness, lies approximately between 0.01 and 1 for the considered cases, which indicates relatively low temperature variations within the wall. Results in terms of inner wall-surface temperatures at

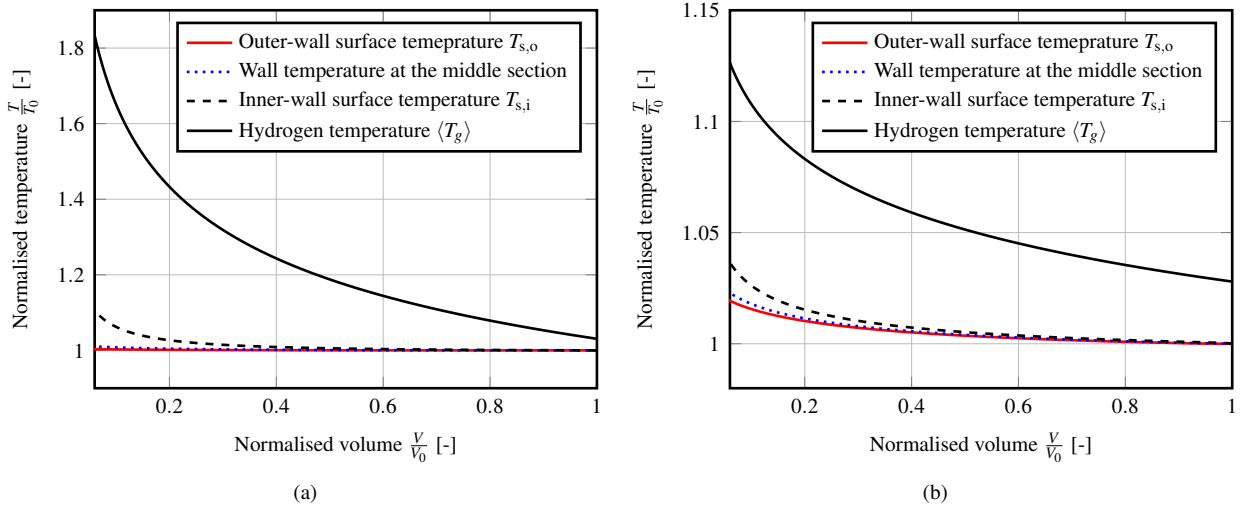


Figure 6: Time-resolved stainless steel wall thermal response, with the outer-wall, inner-wall and mid-section wall temperature evolutions reported along with the hydrogen mass averaged temperature as functions of the normalised gas volume. Results reported here are taken from simulations performed with isothermal walls at 20 °C starting from a static pressure of 15 bar for: (a) a rapid inlet water flowrate  $Q_v = 3$  L/s; and (b) a slow inlet water flowrate  $Q_v = 0.3$  L/s.

the end of the compression stroke are listed in Table 3 for the different cases. Due to its higher thermal conductivity for a similar thermal inertial, the use of AISI P3 allows reduction of the temperature gradient within the wall in comparison to the stainless steel, and thus to reduce the inner-wall surface temperature. Lower temperatures are also observed for the aluminium type, which has a slightly lower thermal inertia than AISI 410, but a thermal conductivity one order of magnitude higher. For the slow compression case, the influence of the wall material is not significant if its thickness is kept at 1 cm. Thickening the wall to 4 cm allows on the contrary an important reduction of the inner-wall thickness temperature. This reduction is also more pronounced for AISI P3 and AL 7068, for which the wall temperature is respectively only 13% and 7% of the final gas temperature. Given its lower density, the Aluminium 7000 series AL 7068 may be a better compromise for reservoir design.

| Material | $Q_v = 3$ L/s        | $Q_v = 0.3$ L/s      | $Q_v = 0.3$ L/s      |
|----------|----------------------|----------------------|----------------------|
|          | $\varepsilon = 1$ cm | $\varepsilon = 1$ cm | $\varepsilon = 4$ cm |
| AISI 410 | 50.3                 | 31.6                 | 28.9                 |
| AISI P3  | 43.2                 | 30.1                 | 22.6                 |
| Al 7068  | 35.9                 | 31.2                 | 24.9                 |

Table 3: Inner wall-surface temperatures (in °C) obtained at the end of compression for different types of wall.

#### 4.2. Influence of initial, operating and thermal boundary conditions

Figure 7 shows the pressure-volume ( $P$ - $V$ ) trace for three different liquid flow rates and thus three different compression times. The ideal isothermal compression is the least demanding in terms of work. The slower the compression process, the closer the  $P$ - $V$  curve to the isothermal reference curve. For a real gas, the isothermal  $P$ - $V$  trace deviates from the straight line of a perfect gas. On the contrary, the adiabatic compression represents an infinitely fast change of state, during which no heat is transferred out of the gas. As for the results obtained at high flow rate, it is interesting to note the relatively low difference of pressure evolution for the two different definition of the wall thermal boundary condition, in comparison to the adiabatic evolution of the same perfect gas. This means that the cooling effect from the liquid-gas interface is more important than the cooling effect from the walls, although the latter has a larger area. This result alleviates the conclusion from Kermani and Rokni [32], and could be explained by the different pressure

ratios between both studies and the absence of the convective effect in the system studied by Kermani and Rokni [32]. Finally, the bulk gas temperature evolutions are shown for the three different liquid flow rates in Figure 8. These results are all obtained with isothermal boundary condition at the wall.

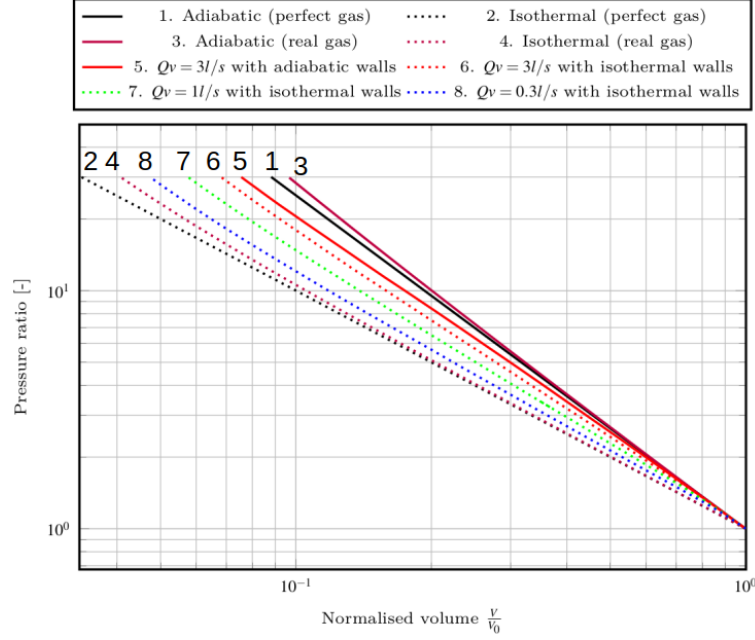


Figure 7: Evolution of the instantaneous pressure ratio for different wall thermal boundary conditions and different flow rates and comparison to the ideal-gas cases. Initial conditions and overall pressure ratio are detailed in Table 2.

Results in terms of compression energy cost, compression efficiency and power density are listed in Table 4. Decreasing the pump flow rate from one order of magnitude allows improvement of the efficiency of the compressor system of 20% for the same parameters. However, this will result in the shrinkage of the power density. High power densities are usually intended, as smaller units are thus required for a given power. As a result, relatively high flow rates are generally chosen and efficiencies are rather improved by maximising the heat transfer during compression (see Section 4.3). As noted qualitatively in Figure 7, the definition of the wall thermal boundary conditions has a relatively low influence on the results. Accounting for isothermal walls does only lead to a 3% reduction in compression efficiency. The compression consumption for the baseline scenario is 1.67kWh/kg, achieving 450 bar. Typical energy consumption for the compression stage of a refueling stations (700 bar) is around 2.43 kWh/kg [48], but it only represents 31% of the total refueling cost [49].

Table 4: Influence of the inlet water flowrate on the compression energy cost, efficiency and power density. Initial conditions, thermal boundary condition and overall pressure ratio are detailed in Table 2. Isothermal compression energy cost is obtained from Eq. (3).

| Model                      | $C_c$ [kWh/kg] | $\eta_c$ [—] | $\dot{w}_c$ [kW/m <sup>3</sup> ] |
|----------------------------|----------------|--------------|----------------------------------|
| $Q_v = 3$ L/s (adia. wall) | 1.75           | 0.68         | 540                              |
| $Q_v = 3$ L/s (iso. wall)  | 1.67           | 0.71         | 536                              |
| $Q_v = 1$ L/s              | 1.52           | 0.78         | 177                              |
| $Q_v = 0.3$ L/s            | 1.30           | 0.91         | 52.5                             |
| Isothermal                 | 1.18           | 1.0          | /                                |

The velocity streamlines in the cylindrical reservoir are shown in Figure 9. As the chamber is empty, the wall temperature gradient leads to the generation of a recirculation zone close to the wall. The recirculation bubble takes then the entire length of the gaseous part. For the high flow rate, the size of recirculation bubble is approximately

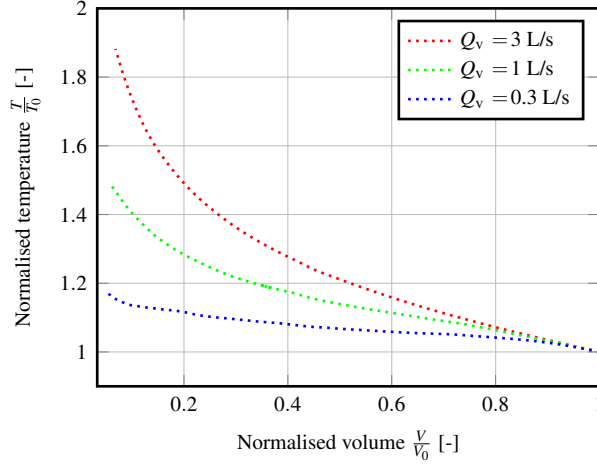


Figure 8: Evolution of the instantaneous bulk gas temperature for different water flow rates, varied from 0.3 to 3 L/s. Initial conditions, wall thermal boundary condition and overall pressure ratio are detailed in Table 2.

$D/5$  in the radial direction. Similar recirculation zones are also present for low flow rates. The hydrogen temperature distribution is non uniform, as the recirculation bubble enhances the cooling effect from the liquid-gas interface. For this reason a slight stratification appears in the axial direction. Local measurements also indicate that the radial thermal boundary layer thickness at the sidewall is similar regardless of the flow rate.

Finally an energy-cost analysis is carried out for different pressure ratios and initial pressure levels. The simulations are performed for the high flow rate and with a ambient temperature as initial temperature. The obtained results are listed in Table 5. For each case, the energy cost is compared to its isothermal equivalent case, from which

Table 5: Influence of the pressure ratio and initial pressure on the compression energy cost, efficiency and temperature at end of the compression stroke. Initial temperature and volume, thermal boundary condition and injection flowrate are kept constant and given in Table 2.

| Model                         | $C_c$ [kWh/kg] | $C_c$ [kWh/kg] isothermal | $\eta_c$ [-] | $T_{end}$ [K] |
|-------------------------------|----------------|---------------------------|--------------|---------------|
| $P_0 = 15$ bar & $r = 30$     | 1.67           | 1.18                      | 0.71         | 552           |
| $P_0 = 15$ bar & $r = 5.48$   | 0.642          | 0.513                     | 0.80         | 413           |
| $P_0 = 82.2$ bar & $r = 5.48$ | 0.652          | 0.549                     | 0.84         | 434           |
| $P_0 = 200$ bar & $r = 5.48$  | 0.737          | 0.631                     | 0.86         | 442           |

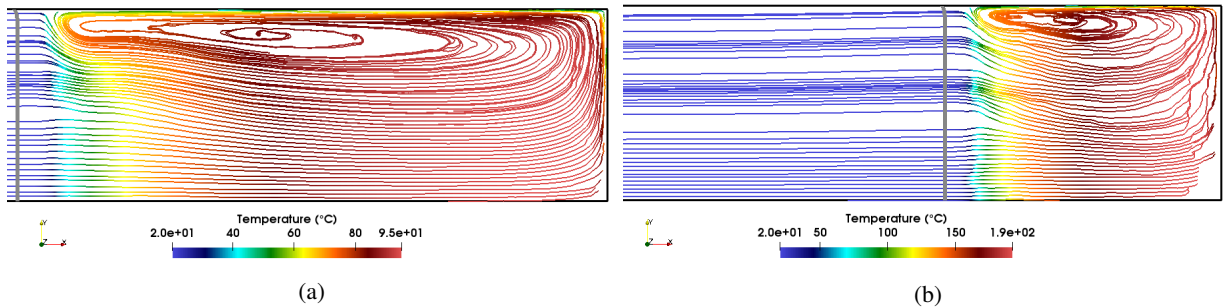


Figure 9: Streamlines in the compression tank coloured by the temperature field reported at two different times of the compression process: (a) at  $t = 5$  s; and (b) at  $t = 8$  s. Results are taken from simulations performed at baseline initial, operating and boundary conditions, as detailed in Table 2. Liquid-gas interface is highlighted as a thick grey line.

the compression efficiency is deduced. As most of the work is performed by the water pump towards the end of the compression, increasing the pressure ratio rapidly increases the energy cost. Uncoupling the compression of hydrogen from 15 to 450 bar by two consecutive half ratios of approximately 5.48 each allows the decrease of the total cost of compression by 0.38 kWh/kg. This 23% reduction in compression energy cost must be compared to the energy cost necessary to cool the hydrogen at ambient temperature before the start of the second compression. Multi-level storage, compression and cooling systems can thus be subject of an optimisation study. This problematic has been investigated by Guo et al. [50] for a diaphragm compressor system. The results highlight also a slight increase of the equivalent isothermal compression consumption when increasing the initial pressure for similar pressure ratios. This is due to the non-ideal behaviour of hydrogen gas at these pressure levels. The increase in the actual compression energy cost is however slower, which leads to a small improvement in compression efficiency.

As for the heat transfer coefficient, its increase rate does not depend on initial pressure. Only the coefficient magnitude increases with initial pressure, due to the higher density and thus thinner thermal boundary layer of the gas. This observation is similar to the one made previously regarding the influence of the compression speed on the heat transfer coefficient.

#### 4.3. Compression energy cost reduction via forced internal convection

In order to mimic the presence of the fan used to create an internal forced convection, a downward momentum source term is added in the compression chamber. This source term is activated within a cylindrical zone between  $0.93H$  and  $0.98H$  of diameter  $5D/6$ . The procedure aims at generating a downward flow in the central part of the reservoir and an upward flow toward the cylinder side wall, as depicted in Figure 10a. The resulting flow enhances thermal mixing, thus increasing the temperature gradients near the cold liner walls and water surface. In addition to these operating conditions, three different volumetric momentum sources terms are considered with the respective following magnitudes:  $25 \text{ N/m}^3$ ;  $250 \text{ N/m}^3$  and  $2500 \text{ N/m}^3$ . These source terms respectively represent a low-speed fan, a medium-speed fan and a high-speed fan, which are named in this manner for the remaining of the paper. The momentum sources are constant in time. For this reason, as the hydrogen density increases during compression, the flow velocity generated by the fan is decreasing over time. As the water is submerging the fan at the very end of the

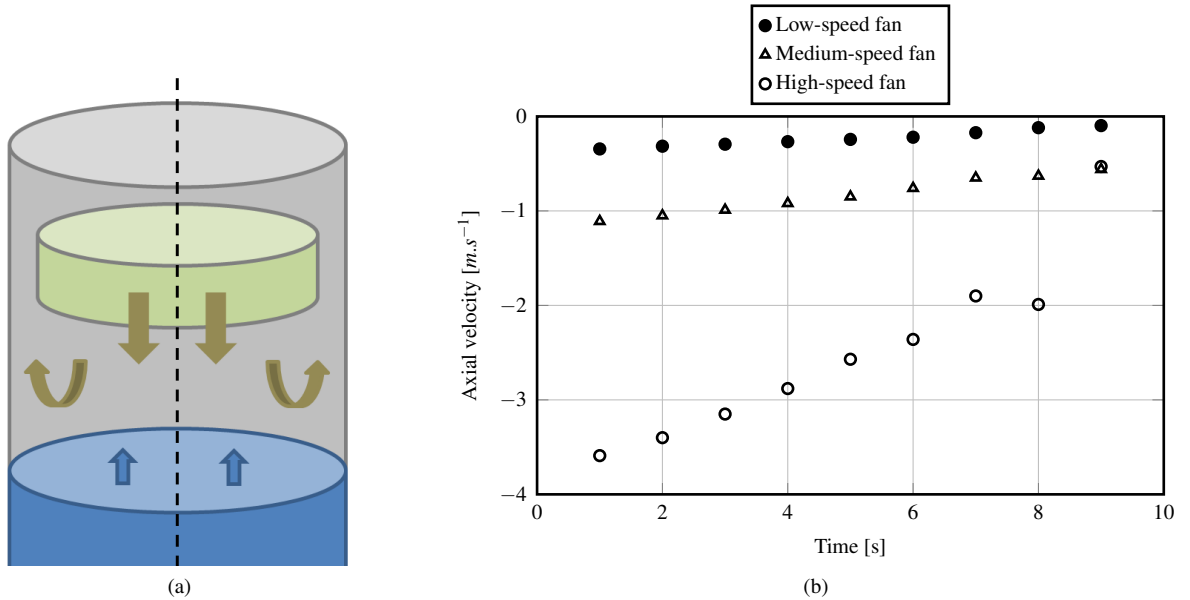
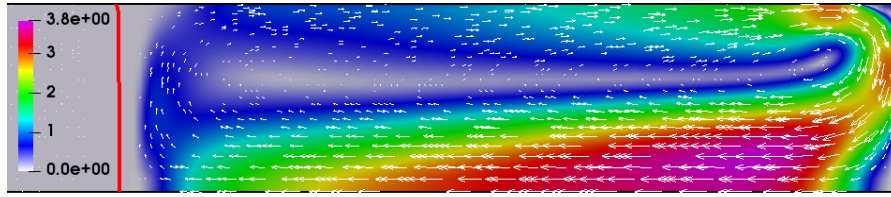
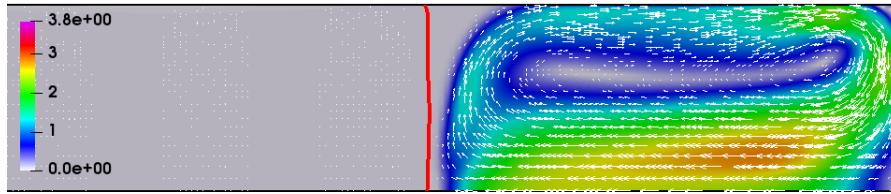


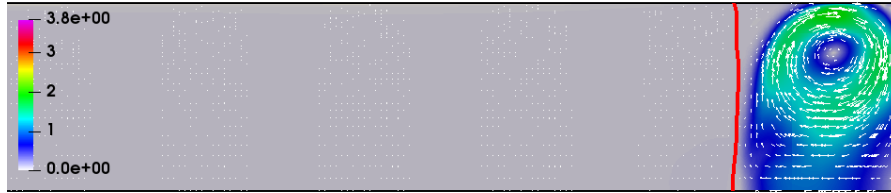
Figure 10: Description and results of the compression energy cost reduction method via forced internal convection: (a) schematics of the downward momentum source applied at the top of the cylindrical tank to simulate the action of an axial fan; (b) Evolution of the average downward axial speed for the three different fan speeds. Results are taken from simulations performed at baseline initial, operating and boundary conditions, as detailed in Table 2.



(a)  $t = 3$  s



(b)  $t = 6$  s



(c)  $t = 9$  s

Figure 11: Velocity vectors of the flow field generated by the medium-speed fan (with contour of the velocity magnitude in the background). Results are taken from simulations performed at baseline initial, operating and boundary conditions, as detailed in Table 2. Liquid-gas interface is highlighted as a thick red line.

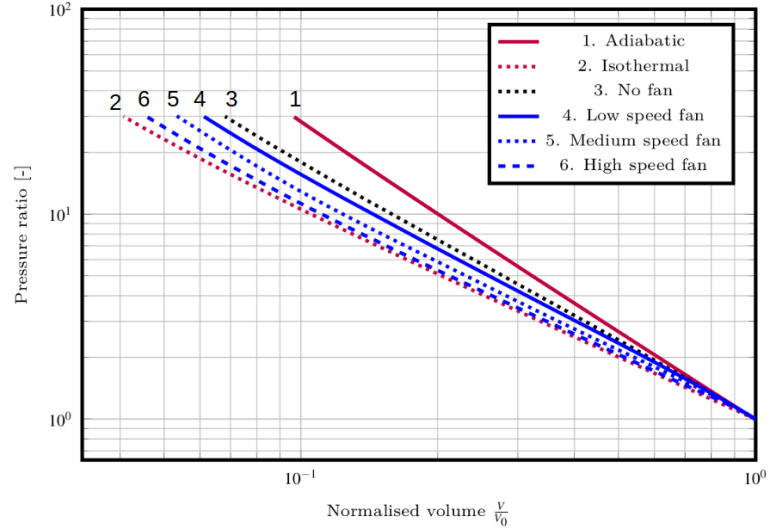


Figure 12: Evolution of the pressure for the three different fans. Results are taken from simulations performed at baseline initial, operating and boundary conditions, as detailed in Table 2.

compression stroke, the gas velocity is ultimately nearly null. The flow velocity evolution is shown in Figure 10b for the three cases, where the time-resolved volume-averaged axial velocity is reported. A difference of two order of magnitude between the momentum sources of the low- and high-speed fans leads to a difference of one order of magnitude in average axial velocity. After 5 s, while an average velocity of 2.6 m/s is obtained with the high-speed fan, the low-speed fan velocity is about 0.24 m/s. The flow pattern is shown in Figure 11 at different times during the compression for the medium-speed fan case. The convection loop takes all the height of the gas layer. Regarding its radial size, although the downward momentum source is enabled in a  $5R/6$  thick zone, the eye of the loop is situated around  $0.7R$ .

The influence of forced convection on the compression stroke is described in Figures 12 and 13. For a similar power density (i.e., fixed inlet water flow rate), increasing the magnitude of the convection loop intensifies heat transfer and reduces the average gas temperature, as shown in Figure 13a. This allows to delay the pressure rise during compression and approach an isothermal process, as shown in Figure 12. The reduction in energy costs with increasing the fan speed is quantified in Table 6. The high-speed fan allows an absolute 24% increase in compression efficiency, i.e., a relative 34% increase. Similar improvements in terms of compression efficiency have been obtained for liquid-piston systems used for compressed air, when inserting porous media [19, 20]. The latter method improves the system performance by increasing the surface area where the heat transfers take place, unlike the approach proposed here which maximizes the internal heat transfer coefficient. Thereby, at approximately  $50 \text{ kW/m}^3$  power density, the use of porous insert increase the compression efficiency from 80% to 97% [19] and from 80% to 92% [20], for an achieved pressure ratio of 10 (rising from atmospheric pressure) and 30 (rising from 7 bar) respectively. For a power density around  $500 \text{ kW/m}^3$ , which corresponds to our baseline case, the compression efficiency is increased from 64% to 86% for the same pressure ratio than our case.

Table 6: Compression energy cost, efficiency and temperature at end of compression for the three different fans. Results are taken from simulations performed at baseline initial, operating and boundary conditions, as detailed in Table 2.

| Model            | $C_c [\text{kWh.kg}^{-1}]$ | $\eta_c [-]$ | $T_{\text{end}} [\text{K}]$ |
|------------------|----------------------------|--------------|-----------------------------|
| No fan           | 1.67                       | 0.71         | 551.7                       |
| Low-speed fan    | 1.52                       | 0.78         | 470.2                       |
| Medium-speed fan | 1.36                       | 0.87         | 395.9                       |
| High-speed fan   | 1.25                       | 0.95         | 331.0                       |

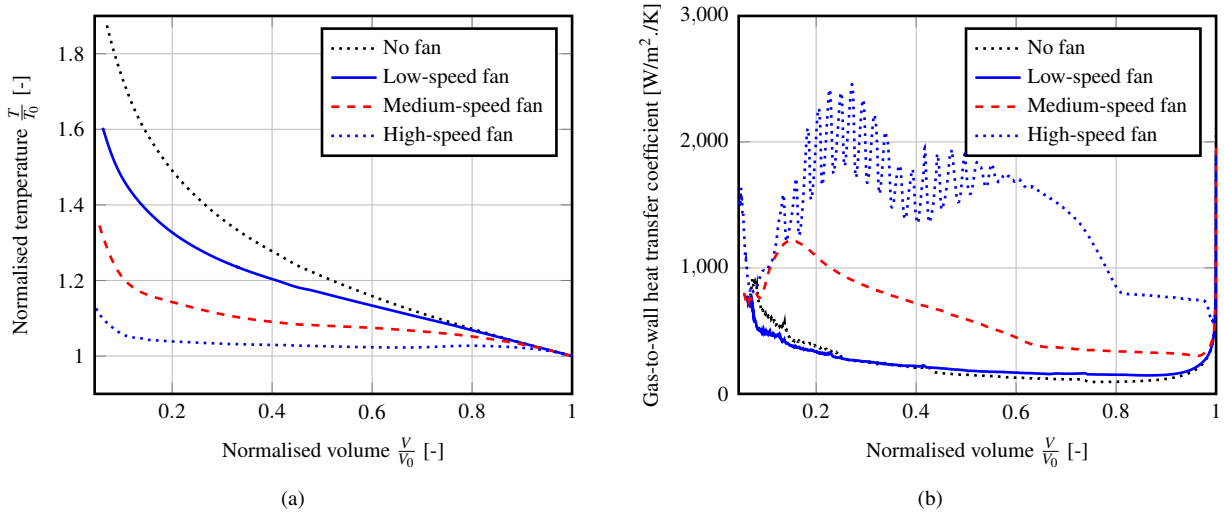


Figure 13: Evolution of: (a) the gas bulk temperature; and (b) the wall heat transfer coefficient for the three different fans. Results are taken from simulations performed at baseline initial, operating and boundary conditions, as detailed in Table 2.

The energy cost for running the fan system is not included here as it is negligible in front of the compression energy cost – the order of magnitude of the latter being 10-100 kW, while the fan power consumption is estimated as <10 W. The shortcomings of such system rather lies on the connectivity and its compatibility with high temperature and pressure, as stated in Section 2.

Figure 13b shows the evolution of the wall heat transfer coefficients for the simulations with fans. The coefficients highlight a similar slope during the first stage of compression. For the higher gas flow rate however, a second phase occurs with higher heat exchange at the walls. The rate of increase of the heat transfer coefficient depends then on the gas flow rate. With the high-speed fan in addition, the wall heat transfer coefficient experiences oscillations during the second half of the compression process. Induced by the detachment and re-attachment of the boundary layer, these oscillations highlight a period of approximately 0.27 s. The decrease of wall heat transfer near the end of the process is the result of the gas flow rate reduction happening when the liquid water reaches the zone where the momentum source is applied.

We have shown how the maximisation of internal heat transfer can lead to a near-isothermal process. In this context, the compression heat is either transferred through the walls or to the water. Assuming most of the heat is passing through the gas-liquid interface, the liquid temperature would only increase from 20°C to approximately 21°C, in mass average, after the first compression stroke. For a continuous operating of the liquid-piston however, this may require an additional external cooling circuit to keep the water temperature at ambient. In the case where a non-negligible part of the heat is transferred through the walls, external heat transfer can be enhanced as well to keep a near-isothermal wall boundary condition. The increase of the external heat transfer can be similarly obtained with fans for instance.

## 5. Conclusions

A liquid-piston system has been presented in this paper for hydrogen applications in the automotive industry. In the specific context of hydrogen-driven vehicles, high-pressure tanks are key to provide substantial range. The development of cost-effective compression, storage and dispensing (CSD) hydrogen stations is thus a crucial challenge for the uptake of hydrogen-powered transportation, as this requires hydrogen to be compressed rapidly over high pressure ratios while minimising heat production in order to deliver hydrogen at a near-ambient temperature and reduce the compression work. In this paper, the thermodynamic performance of an intermediary-stage liquid-piston compressor – bringing hydrogen gas from 15 bar to 450 bar – has been investigated through axi-symmetric dynamic

simulations, whereby the two-phase thermofluid problem was solved using VOF (volume of fluid) methods, a real gas model for the gaseous phase and with isothermal-wall boundary conditions. The behaviour of compressed hydrogen gas and the efficiency of this system has been analysed for high pressure ratios up to 30. Simulations were performed with ANSYS Fluent v15.

A qualitative and quantitative analysis of the unsteady conjugate gas-to-wall heat transfer has been proposed, both to explain the infinite values of the heat transfer coefficient (as defined in the Newton's law of cooling) at the beginning of the compression stroke, and to derive accurate complex Nusselt correlations that capture this initial singularity. The complex Nusselt-Peclet correlation fictitiously accounts for heat accumulation within the thermal boundary layer. The latter have been measured and used to verify *a posteriori* the isothermal-wall assumption of the CFD model. This thermal condition remain reasonable for the considered scenarios, depending on the wall material used. Using aluminium 7068 seem the best option to keep a quasi-isothermal condition at the wall, while having both sufficient mechanical resistance and low weight.

In the baseline configuration, a 71-% compression efficiency (defined as the ratio of the compression work of a fictive isothermal process to the actual compression work) is obtained to compress approximately 40 g of hydrogen gas from 15 to 450 bar in about 10 s, i.e. with a water inlet flowrate of 3 L/s. This corresponds to a compression energy cost, defined as the ratio of the total work required to compress hydrogen to the mass of gas, of 1.67 kWh/kg.

In the second part of the study, the potential of heat transfer enhancement through forced convection during the compression process has been investigated. Assuming that the walls remain isothermal during the compression stroke, a significant pumping work reduction can be achieved thanks to a quasi-isothermal compression. For a similar power density (i.e., fixed inlet water flow rate of 3 L/s), increasing the magnitude of the convection loop intensifies heat transfer. By imposing a volumetric momentum source of 2500 N/m<sup>3</sup> in the top part of the compression chamber, the compression consumption is reduced down to 1.25 kWh/kg and the compression efficiency reaches 95%, with a hydrogen temperature at the end of the compression stroke of only 58 °C. This shows that gas-to-wall heat transfer enhancement through forced in-cylinder convection has the potential to reach near-isothermal compression. This corresponds to a 25-% decrease in compression energy cost and an absolute 24-% increase in compression efficiency when compared to the baseline fanless configuration.

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## References

- [1] Global energy-related CO<sub>2</sub> emissions by sector, Tech. rep., International Energy Agency (IEA) (2021). URL <https://www.iea.org/data-and-statistics/charts/global-energy-related-co2-emissions-by-sector>
- [2] C. Thomas, Fuel cell and battery electric vehicles compared, International Journal of Hydrogen Energy 34 (15) (2009) 6005–6020. doi:10.1016/j.ijhydene.2009.06.003.
- [3] M. Saadat, P. Y. Li, T. W. Simon, Optimal trajectories for a liquid piston compressor/expander in a Compressed Air Energy Storage system with consideration of heat transfer and friction, in: Proceedings of the American Control Conference, 2012. doi:10.1109/acc.2012.6315616.
- [4] P. Y. Li, M. Saadat, An approach to reduce the flow requirement for a liquid piston near-isothermal air compressor/expander in a compressed air energy storage system, IET Renewable Power Generation 10 (10) (2016) 1506–1514. doi:10.1049/iet-rpg.2016.0055.
- [5] M. Saadat, Modeling, control and optimization of a novel compressed air energy storage system for off-shore wind turbines, PhD Thesis, University of Minnesota (2016).
- [6] A. M. Pantaleo, M. Simpson, G. Rotolo, E. Distaso, O. A. Oyewunmi, P. Sapin, P. De Palma, C. N. Markides, Thermoeconomic optimisation of small-scale organic rankine cycle systems based on screw vs. piston expander maps in waste heat recovery applications, Energy Conversion and Management 200 (2019) 112053. doi:10.1016/j.enconman.2019.112053.
- [7] M. A. Chatzopoulou, M. Simpson, P. Sapin, C. N. Markides, Off-design optimisation of organic rankine cycle (orc) engines with piston expanders for medium-scale combined heat and power applications, Applied energy 238 (2019) 1211–1236. doi:10.1016/j.apenergy.2018.12.086.
- [8] A. J. White, G. Parks, C. N. Markides, Thermodynamic analysis of pumped thermal electricity storage, Applied Thermal Engineering 53 (2) (2013) 291–298. doi:10.1016/j.applthermaleng.2012.03.030.

- [9] J. D. Van de Ven, P. Y. Li, Liquid piston gas compression, *Applied Energy* 86 (10) (2009) 2183–2191. doi:10.1016/j.apenergy.2008.12.001.
- [10] V. C. Patil, P. Acharya, P. I. Ro, Experimental investigation of heat transfer in liquid piston compressor, *Applied Thermal Engineering* 146 (June 2018) (2019) 169–179. doi:10.1016/j.applthermaleng.2018.09.121.
- [11] V. Shcherba, E. Nosov, E. Pavlyuchenko, I. Bulgakova, Approximation of the compression process to isothermal in a reciprocating compressor with a liquid piston, *Applied Thermal Engineering* 207 (August 2021) (2022) 118151. doi:10.1016/j.applthermaleng.2022.118151. URL <https://doi.org/10.1016/j.applthermaleng.2022.118151>
- [12] A. Mazzucco, E. Rothuizen, J. E. Jørgensen, T. R. Jensen, M. Rokni, Integration of phase change materials in compressed hydrogen gas systems: Modelling and parametric analysis, *International Journal of Hydrogen Energy* 41 (2) (2016) 1060–1073. doi:10.1016/j.ijhydene.2015.09.034.
- [13] A. Srivatsa, P. Y. Li, How moisture content affects the performance of a liquid piston air compressor/expander, *Journal of Energy Storage* 18 (2018) 121–132. doi:10.1016/j.est.2018.04.017.
- [14] V. C. Patil, P. I. Ro, Experimental study of heat transfer enhancement in liquid piston compressor using aqueous foam, *Applied Thermal Engineering* 164 (March 2019) (2020) 114441. doi:10.1016/j.applthermaleng.2019.114441. URL <https://doi.org/10.1016/j.applthermaleng.2019.114441>
- [15] C. Qin, E. Loth, Simulation of spray direct injection for compressed air energy storage, *Applied Thermal Engineering* 95 (2016) 24–34. doi:10.1016/j.applthermaleng.2015.11.008. URL <http://dx.doi.org/10.1016/j.applthermaleng.2015.11.008>
- [16] C. Qin, E. Loth, Liquid piston compression efficiency with droplet heat transfer, *Applied Energy* 114 (2014) 539–550. doi:10.1016/j.apenergy.2013.10.005.
- [17] S. K. Khaitan, M. Raju, J. D. McCalley, Design of a novel and efficient hydrogen compressor for wind energy based storage systems, *International Journal of Hydrogen Energy* 40 (3) (2015) 1379–1387. doi:10.1016/j.ijhydene.2014.11.066.
- [18] P. Sapin, M. Simpson, C. Kirmse, C. N. Markides, Dynamic modelling of water-droplet spray injection in reciprocating-piston compressors, in: *Proceedings of the 31st International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems (ECOS)*, 2018.
- [19] B. Yan, J. Wieberdink, F. Shirazi, P. Y. Li, T. W. Simon, J. D. Van de Ven, Experimental study of heat transfer enhancement in a liquid piston compressor/expander using porous media inserts, *Applied Energy* 154 (2015) 40–50. doi:10.1016/j.apenergy.2015.04.106.
- [20] J. Wieberdink, P. Y. Li, T. W. Simon, J. D. Van de Ven, Effects of porous media insert on the efficiency and power density of a high pressure (210 bar) liquid piston air compressor/expander – An experimental study, *Applied Energy* 212 (August 2017) (2018) 1025–1037. doi:10.1016/j.apenergy.2017.12.093.
- [21] M. Saadat, P. Y. Li, Modeling and control of a novel compressed air energy storage system for offshore wind turbine, in: *Proceedings of the American Control Conference*, 2012, pp. 3032–3037. doi:10.1109/acc.2012.6315575.
- [22] C. Zhang, B. Yan, J. Wieberdink, P. Y. Li, J. D. Van De Ven, E. Loth, T. W. Simon, Thermal analysis of a compressor for application to Compressed Air Energy Storage, *Applied Thermal Engineering* 73 (2) (2014) 1402–1411. doi:10.1016/j.applthermaleng.2014.08.014.
- [23] C. Zhang, J. Wieberdink, T. W. Simon, P. Y. Li, J. Van De Ven, E. Loth, Numerical analysis of heat exchangers used in a liquid piston compressor using a one-dimensional model with an embedded two-dimensional submodel, in: *Proceedings of the ASME International Mechanical Engineering Congress and Exposition (IMECE)*, 2014. doi:10.1115/IMECE2014-38567.
- [24] C. Zhang, P. Y. Li, J. D. Van De Ven, T. W. Simon, Design analysis of a liquid-piston compression chamber with application to compressed air energy storage, *Applied Thermal Engineering* 101 (2016) 704–709. doi:10.1016/j.applthermaleng.2016.01.082.
- [25] M. C. Galassi, D. Baraldi, B. Acosta Iborra, P. Moretto, CFD analysis of fast filling scenarios for 70 MPa hydrogen type IV tanks, *International Journal of Hydrogen Energy* 37 (8) (2012) 6886–6892. doi:10.1016/j.ijhydene.2012.01.041.
- [26] M. C. Galassi, E. Papanikolaou, M. Heitsch, D. Baraldi, B. A. Iborra, P. Moretto, Assessment of CFD models for hydrogen fast filling simulations, *International Journal of Hydrogen Energy* 39 (11) (2014) 6252–6260. doi:10.1016/j.ijhydene.2013.03.164.
- [27] D. Melideo, D. Baraldi, M. C. Galassi, R. Ortiz Cebolla, B. Acosta Iborra, P. Moretto, CFD model performance benchmark of fast filling simulations of hydrogen tanks with pre-cooling, *International Journal of Hydrogen Energy* 39 (9) (2014) 4389–4395. doi:10.1016/j.ijhydene.2013.12.196.
- [28] I. Simonovski, D. Baraldi, D. Melideo, B. Acosta-Iborra, Thermal simulations of a hydrogen storage tank during fast filling, *International Journal of Hydrogen Energy* 40 (36) (2015) 12560–12571. doi:10.1016/j.ijhydene.2015.06.114.
- [29] D. Melideo, D. Baraldi, CFD analysis of fast filling strategies for hydrogen tanks and their effects on key-parameters, *International Journal of Hydrogen Energy* 40 (1) (2015) 735–745. doi:10.1016/j.ijhydene.2014.10.138.
- [30] D. Melideo, D. Baraldi, B. Acosta-Iborra, R. Ortiz Cebolla, P. Moretto, CFD simulations of filling and emptying of hydrogen tanks, *International Journal of Hydrogen Energy* 42 (11) (2017) 7304–7313. doi:10.1016/j.ijhydene.2016.05.262.
- [31] Y. Wang, X. Dai, H. You, M. Gao, Research on the design of hydrogen supply system of 70 MPa hydrogen storage cylinder for vehicles, *International Journal of Hydrogen Energy* 43 (41) (2018) 19189–19195. doi:10.1016/j.ijhydene.2018.08.138.
- [32] N. A. Kermani, M. Rokni, Heat transfer analysis of liquid piston compressor for hydrogen applications, *International Journal of Hydrogen Energy* 40 (35) (2015) 11522–11529. doi:10.1016/j.ijhydene.2015.01.098.
- [33] I. H. Bell, J. Wronski, S. Quoilin, V. Lemort, Pure and pseudo-pure fluid thermophysical property evaluation and the open-source thermophysical property library coolprop, *Industrial and Engineering Chemistry Research* 53 (6) (2014) 2498–2508. doi:10.1021/ie4033999.
- [34] H. Pfriem, Periodic heat transfer at small pressure fluctuations, *Tech. rep.*, NACA TM-1048 (1943).
- [35] K. Lee, A simplistic model of cyclic heat transfer phenomena in closed spaces, in: *Proceedings of the Eighteenth Intersociety Energy Conversion Engineering Conference*, Vol. 2, 1983, pp. 720–723.
- [36] A. A. Kornhauser, J. L. Smith, Application of a complex nusselt number to heat transfer during compression and expansion, *Journal of Heat Transfer* 116 (3) (1994) 536–542. doi:10.1115/1.2910904.
- [37] P. Sapin, A. Taleb, C. Barfuss, A. J. White, D. Fabris, C. N. Markides, Thermodynamic losses in a gas spring: Comparison of experimental and

- numerical results, in: Proceedings of the 12th International Conference on Heat Transfer Fluid Mechanics and Thermodynamics (HEFAT), 2016.
- [38] U. Lekic, J. B. Kok, Heat Transfer and Fluid Flows in Gas Springs, *The Open Thermodynamics Journal* 4 (1) (2010) 13–26. doi:10.2174/1874396x01004010013.
  - [39] R. Mathie, C. N. Markides, A. J. White, A framework for the analysis of thermal losses in reciprocating compressors and expanders, *Heat Transfer Engineering* 35 (16-17) (2014) 1435–1449. doi:10.1080/01457632.2014.889460.
  - [40] U. Lekić, Fluid flow and heat transfer in a helium gas spring, Ph.D. thesis, University of Twente (2011).
  - [41] C. Willich, C. N. Markides, A. J. White, An investigation of heat transfer losses in reciprocating devices, *Applied Thermal Engineering* 111 (2017) 903–913. doi:10.1016/j.applthermaleng.2016.09.136.
  - [42] D.-Y. Peng, D. B. Robinson, A new two-constant equation of state, *Industrial & Engineering Chemistry Fundamentals* 15 (1) (1976) 59–64. doi:10.1021/i160057a011.
  - [43] B. McBride, S. Gordon, M. Reno, Coefficients for Calculating Thermodynamic and Transport Properties of Individual Species, Nasa Technical Memorandum 4513 (NASA-TM-4513) (1993) 98.  
URL [http://ntrs.nasa.gov/archive/nasa/casi.ntrs.nasa.gov/19940013151\\_1994013151.pdf](http://ntrs.nasa.gov/archive/nasa/casi.ntrs.nasa.gov/19940013151_1994013151.pdf)
  - [44] ANSYS Fluent Theory Guide, Tech. Rep. November (2013).
  - [45] S. C. Kim, S. H. Lee, K. B. Yoon, Thermal characteristics during hydrogen fueling process of type IV cylinder, *International Journal of Hydrogen Energy* 35 (13) (2010) 6830–6835. doi:10.1016/j.ijhydene.2010.03.130.
  - [46] A. G. E. software 21.2.0, Ansys, inc., cambridge, uk, 2021 ([www.ansys.com/materials](http://www.ansys.com/materials)).
  - [47] ISO 9809-1:2019: Gas cylinders - Design, construction and testing of refillable seamless steel gas cylinders and tubes - Part 1: Quenched and tempered steel cylinders and tubes with tensile strength less than 1 100 MPa, Standard, International Organization for Standardization, Geneva, CH (Oct. 2019).
  - [48] A. Bauer, T. Mayer, M. Semmel, M. A. Guerrero Morales, J. Wind, Energetic evaluation of hydrogen refueling stations with liquid or gaseous stored hydrogen, *International Journal of Hydrogen Energy* 44 (13) (2019) 6795–6812. doi:10.1016/j.ijhydene.2019.01.087.  
URL <https://doi.org/10.1016/j.ijhydene.2019.01.087>
  - [49] S. S. Bhogilla, H. Niyas, Design of a hydrogen compressor for hydrogen fueling stations, *International Journal of Hydrogen Energy* 44 (55) (2019) 29329–29337. doi:10.1016/j.ijhydene.2019.02.171.  
URL <https://doi.org/10.1016/j.ijhydene.2019.02.171>
  - [50] J. Guo, L. Xing, Z. Hua, C. Gu, J. Zheng, Optimization of compressed hydrogen gas cycling test system based on multi-stage storage and self-pressurized method, *International Journal of Hydrogen Energy* 41 (36) (2016) 16306–16315. doi:10.1016/j.ijhydene.2016.05.076.