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Thermal Analysis of a Hydrogen Bulk Gas Transport System

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Abstract – Hydrogen bulk gas transport (BGT) systems are needed to provide efficient movement of carbon-free energy. This study considers containerised or trailer-mounted BGT systems comprising an array of high-pressure hydrogen cylinders. Rapid filling of such cylinders leads to large changes in gas temperature which may exceed the maximum temperature limit of the cylinder materials. Therefore the filling rate is limited by the rate at which heat can be dissipated from the cylinder. This study develops, validates and applies low-dimensional models for the thermal response of hydrogen cylinder arrays, characterising how different design choices affect the minimum filling time for BGT systems subject only to natural convection. Validity of the low-dimensional modelling is supported by comparison with three-dimensional computational fluid dynamic simulations. This study considers BGT systems with vertically-oriented cylinders and analyses the effects of inline or staggered arrangements of cylinders, cylinder diameter, cylinder spacing, and fill rate. It is found that the BGT system filling rate is limited primarily by convective heat transfer from the outer cylinder walls. Heat transfer tends to improve for systems with smaller cylinder diameter and larger cylinder spacing. The heat transfer rate is greatest for widely-spaced staggered cylinder arrangements, however close-packed arrangements provide a better compromise between overall storage density and fill time.

Keywords**:** hydrogen storage; bulk gas transport; array of cylinders; heat transfer

1. Introduction

Hydrogen is a potential carbon-free energy carrier for transport and industrial applications where direct electrification is not feasible. In the absence of appropriate pipe networks or on-site production, hydrogen bulk gas transport (BGT) systems are needed to deliver hydrogen to where it is to be stored, used, or dispensed to vehicles. BGT systems are mobile containers or trailers comprising several high-pressure gas cylinders bundled together. Traditional "tube trailers" have used steel cylinders with a high net weight, which can lead to mass-related transport restrictions. The newest BGT concepts, as illustrated in Fig. 1, use lighter composite cylinders [1, 2] rated to over 300 bar to increase both gravimetric and volumetric gravimetric energy density. In addition to energy density, the time and energy taken to fill or empty the BGT system are important aspects of operational performance.

During filling, pressurisation of the gas within the cylinder leads to a temperature rise. The SAE TIR J2601 standard specifies a maximum gas temperature of 85°C for composite cylinders used for light duty hydrogen vehicles [3], however lower temperature limits, of perhaps 65°C, might be specified for heavy-duty BGT applications. In the case of very rapid near-adiabatic filling of a cylinder, the gas temperature could greatly exceed the maximum allowable temperature. The rate at which the cylinder can be filled therefore is limited by the need to dissipate heat from the gas during filling. Since it is desirable to fill automotive fuel tanks within around three minutes, to avoid inconveniencing the waiting customer, a large body of applied research activity has addressed heat transfer aspects of fast filling hydrogen vehicles. Through experimental characterisation [4] and computational fluid dynamic studies [5], low-dimensional models have been developed that accurately predict the thermal response of many hydrogen cylinders during rapid filling by considering convective heat transfer from the hydrogen into the cylinder's structure and the thermal diffusion within the solid structure [6, 7].

Fig. 1: Illustration of a containerised Bulk Gas Transport system with vertically-oriented cylinders in a staggered array.

The characteristic timescale for thermal diffusion through the composite cylinder[1] is typically greater than the three minute fill duration of a hydrogen vehicle, so external transfer of heat from the cylinder to the environment has limited influence. Instead, fast filling of hydrogen vehicles requires pre-cooling of the hydrogen before dispensing it to the vehicle [8], incurring a significant cost. In contrast, a longer fill time may be tolerated for a BGT system compared to a passenger vehicle, providing time for external heat rejection and potentially avoiding the need to pre-cool the hydrogen.

The filling time of a BGT system without pre-cooling is constrained by the rate at which heat is rejected to the environment. The present study is restricted to BGT systems that rely on passive cooling by natural convection. The main design choices affecting external heat rejection are expected to include the diameter and spacing of the cylinders, whether the cylinders are oriented horizontally or vertically, and whether the cylinders are packed in an inline or staggered arrangement. To design the BGT system with an acceptably short fill time, we require a proper understanding of how various design choices affect the heat rejection rate. It is therefore necessary to extend the understanding and thermal modelling of cylinder filling, established previously in the context of fast fill of hydrogen vehicles, to take account of external heat rejection in cylinder arrays.

This report proceeds by setting out the formulation of a low-dimensional thermal model for an idealised array of cylinders that permits rapid simulation of various filling scenarios for each system design. The validity of the model is assessed by comparison with three-dimensional computational fluid dynamic simulations for the cylinder array. Subsequently the thermal model is used to analyse the impact of the major design and operating choices on thermal performance.

2. Model formulation

The objectives of this study are to develop an efficient low-dimensional thermal model that is applicable to a wide range of different BGT concepts, and then to use the model to characterise how the main design choices impact heat rejection and fill time. We consider a range of idealised BGT designs that fit within the envelope of a standard forty-foot intermodal container. The proposed BGT system is rated to 350 barg at 15 °C, and operates with gas temperatures up to 65 °C. It is assumed that the sides of the container are enclosed, but air is free to flow into/out of the top and bottom of the container.

[1] The characteristic timescale for thermal diffusion through a carbon fibre-reinforced plastic cylinder wall with thickness l of 2.4 cm and thermal diffusivity α of 8.94×10^{-7} m^{2}s^{-1} is estimated by $\tau = l^2/\alpha$ as around 10 minutes.

The cylinders are arranged either in line with one another, forming a square grid when viewed end-on, or arranged in a staggered array, forming a grid of equilateral triangles when viewed end-on. This study presents modelling for the case where the cylinders are aligned with the vertical axis of the container, with 2.338 m long cylinders to allow space for end fittings. The system shown in Fig. 1 depicts an example of a vertically-aligned staggered configuration.

The spacing S between cylinders is defined as the distance between the centres of two adjacent cylinders. The cylinder spacing and outer diameter D then determine the number of cylinders that fit within a bounding box of 11.5 m × 2.3 m × 2.338 m, allowing space for piping and framework within the envelope of a 40 foot ISO container. We model the cylinders as straight-edged cylinders with hemispherical ends, and 0.3, 0.4, 0.5 or 0.6 m outer diameter. The cylinders are assumed to be constructed with a 5 mm thick plastic liner, wrapped in a carbon fibre-reinforced plastic (CFRP) laminate with 24 mm thickness. The specifications approximate those of commercially available Type IV (plastic lined) CFRP composite cylinders. Since the thermal resistance of the cylinder structure is secondary to the thermal resistance of external convection, small differences in cylinder design do not affect the conclusions of this study.

In order to develop a simple and time-efficient computational prediction of the maximum gas temperature within the system, we consider the temperature within a single cylinder near the centre of the cylinder array, where the cooling flow of air is most restricted. At this inner location, the flow is largely unaffected by transverse flow and heat transfer at the edges of the array and we assume that the flow around the cylinder is periodic in the horizontal directions.

The model employs an unsteady lumped approach, assuming that the hydrogen gas has spatially-uniform time-varying temperature and pressure inside the cylinder. The cylinder wall is approximated as having uniform thickness and heat flux over its surface area, with a one-dimensional temperature profile in the wall-normal direction. New modelling is then developed for the heat transfer coefficient between the outside wall and the environment to account for effect of the geometry of the cylinder array on the external heat transfer.

2.1. Governing equations

The rate of change of the internal energy of the hydrogen in cylinder U_{H_2} is equal to the rate of stagnation enthalpy entering the cylinder, $h_{0,in}\dot{m}_{in}$, plus the rate of heat transfer into the hydrogen from the inner cylinder wall, $\dot{Q}_1$.

$$\frac{dU_{H_2}}{dt} = h_{0,in}\,\dot{m}_{in} + \dot{Q}_1 \tag{1}$$

Due to the high pressure and density inside a full cylinder, the model accounts for real gas effects by calculating thermodynamic and transport properties of normal hydrogen using the CoolProp software library [9].

Neglecting surface curvature effects, one-dimensional conduction through the cylinder wall is governed by

$$\frac{\partial T_w}{\partial t} = \frac{1}{\rho_w c_{p,w}}\frac{\partial}{\partial x}\left(k_w\frac{\partial T_w}{\partial x}\right), \tag{2}$$

where $c_{p,w}$, ρ_w and k_w are the isobaric specific heat capacity, density and thermal conductivity of the cylinder wall material, equal to 1.58 kJ.kg^{-1}.K^{-1}, 1286 kg.m^{-3}, 1.17 W.m^{-1}.K^{-1} in the liner and 0.94 kJ.kg^{-1}.K^{-1}, 1550 kg.m^{-3}, 1.3 W.m^{-1}.K^{-1} in the CFRP laminate. The heat flux at the inner surface of the cylinder x_1 is modelled with heat transfer coefficient $h_{X,1}$ and surface area $A_1$by

$$\dot{Q}_1 = k_w A_1 \frac{\partial T_w}{\partial x}\bigg|_{x_1} = h_{X,1} A_1 \big(T_w(x_1) - T_{H_2}\big). \tag{3}$$

The heat flux at the outer surface of the cylinder x_2 is modelled with heat transfer coefficient $h_{X,2}$ and surface area A_2 by

$$-k_w A_2 \frac{\partial T_w}{\partial x}\bigg|_{x_2} = h_{X,2} A_2 (T_w(x_2) - T_\infty). \tag{4}$$

For consistency with Eq. (dT/dx), we approximate $A_2 = A_1 = \pi LD$, where L is the overall cylinder length and D is the cylinder diameter.

2.2. Internal convective heat transfer

The flow within the cylinder is driven primarily by the momentum of the injected hydrogen [7]. Injection of a d_j diameter jet of hydrogen with velocity V_j along the centreline of the cylinder sets up a toroidal flow recirculation that extends axially around 3.5 diameters into the cylinder [7]. Within the recirculation region, the forced convection Nusselt number scales with the jet Reynolds number $Re_j = d_j V_j / \nu_{H_2}$ and is modelled as [7]

$$Nu_f' = 0.0136 Re_{jet}^{0.95}. \tag{5}$$

The hydrogen inlet pipe is assumed to have diameter $d_j = 0.025$ m and the jet velocity is calculated from the imposed stagnation properties and mass flow through the inlet nozzle.

Cylinders used for BGT systems are typically more than 3.5 diameters long. The heat transfer rate is substantially lower in the non-recirculating end zone [7], and the overall forced convection Nusselt number for the whole cylinder is estimated to be [7]

$$\frac{h_f D}{k_{H_2}} = Nu_f = Nu_f' \times \min\left(1, \frac{3.5}{(L/D)}\right). \tag{6}$$

For low injection rates, the effect of internal natural convection needs to be taken into account. The heat transfer coefficient for natural convection is modelled as [7]

$$h_n = 0.104 \frac{k_{H_2}}{D} Ra^{0.352}. \tag{7}$$

The Rayleigh number, Ra, is calculated using the value of acceleration due to gravity, g, the fluid's coefficient of thermal expansion, β, the temperature difference between the cylinder wall and the fluid, $T_{wall} - T_{fluid}$, the length scale, l, the fluid's kinematic viscosity, ν, and the fluids thermal diffusivity, α

$$Ra = \left|\frac{\left(g\beta\left(T_w - T_{fluid}\right) l^3\right)}{\nu\alpha}\right|. \tag{8}$$

The length scale is taken as the cylinder length. The contributions of forced and natural internal convection are taken into account by

$$h_{X,1} = \left(h_f^4 + h_n^4\right)^{\frac{1}{4}}. \tag{9}$$

2.3. External convective heat transfer

To get the worst-case cylinder temperature, we model a cylinder near the middle of the array and consider the buoyancy-driven upward flow of air through a unit cell of the array. In the absence of heat transfer measurements for arrays of large vertically-oriented cylinders, the average Nusselt number for the channel between adjacent cylinders is estimated using the empirical model for natural convection around isothermal parallel plates given by Badr et al. [10]

$$\overline{Nu}_T = 0.64(Ra_b\, b/L)^{0.27} \tag{10}$$

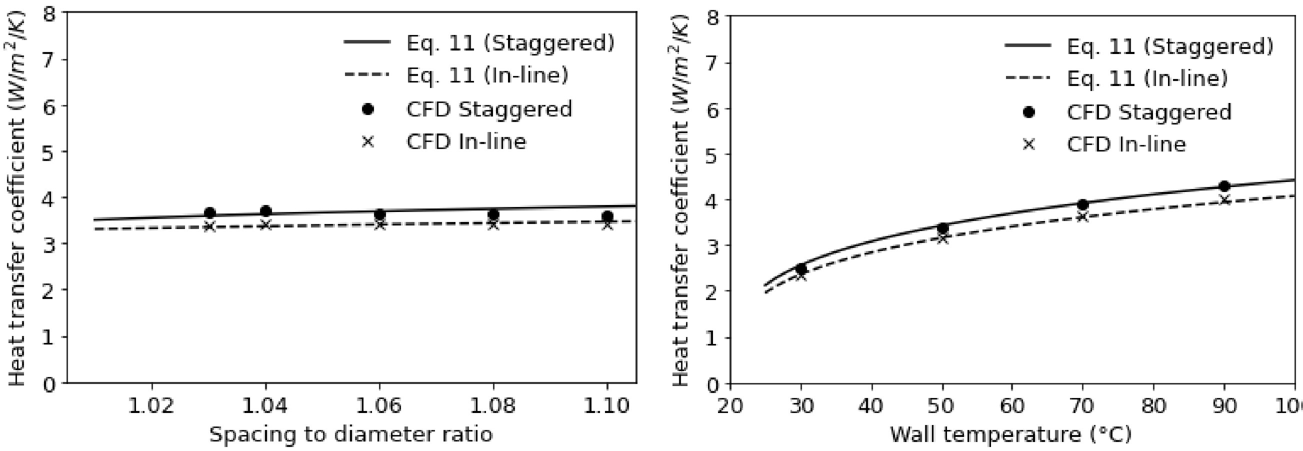
where the Nusselt and Rayleigh numbers are specified using the plate spacing b (half of the hydraulic diameter of the channel between adjacent cylinders) as length scale.

The ability of Eq. 10 to predict heat transfer in an array of vertical cylinders has been assessed by performing three-dimensional CFD of a unit cell of inline and staggered arrays for a cylinder with 2.5 m length and 4.5 length to diameter ratio. The ambient temperature is 20℃ and a constant wall temperature is imposed. The transitional/turbulent flow is simulated by the low Reynolds number k-ε Reynolds Averaged Navier Stokes model and the Boussinesq approximation for density variation is implemented in Fluent version 2022 R2. Due to the multiple symmetries in the array, a three-dimensional domain consisting of a one eighth segment of a cylinder is simulated for an inline array (one twelfth segment for staggered array), employing symmetry conditions as required. The geometry is meshed using an inflation layer on the cylinder surface, and an unstructured mesh elsewhere. The simulation approach has been verified by demonstrating that results are numerically converged with respect to grid spacing and solver tolerances. The choice of mathematical models has been validated by prediction of relevant natural convection problems, including heat transfer from an isolated vertical cylinder [11], yielding predictions of average Nusselt number typically within 10% of empirical correlations.

The heat transfer rates predicted by the CFD model are shown in Fig. 2 for a range of cylinder spacing values S/D between 1.03 and 1.10 and a range of wall temperature between 25℃ and 90℃. Assuming that the functional form of Eq. 10 applies also to arrays of vertical cylinders, agreement with the CFD data is improved by use of

$$\overline{Nu}_T = \begin{cases} 0.58(Ra_b\, b/L)^{0.27}\,; Staggered \\ 0.51(Ra_b\, b/L)^{0.27}; Inline \end{cases} \tag{11}$$

The model presented in Eq. 11 may be improved further as heat transfer data relevant to BGT systems becomes publicly available, however it serves as a reasonable approximation for the present assessment of the effects of the main design variables.



(a) (b)

Fig. 2 Variations in the external heat transfer coefficient with (a) spacing to diameter ratio keeping wall temperature as 60℃ and (b) wall temperature for inline and staggered arrays of cylinders keeping spacing to diameter ratio as 1.06.

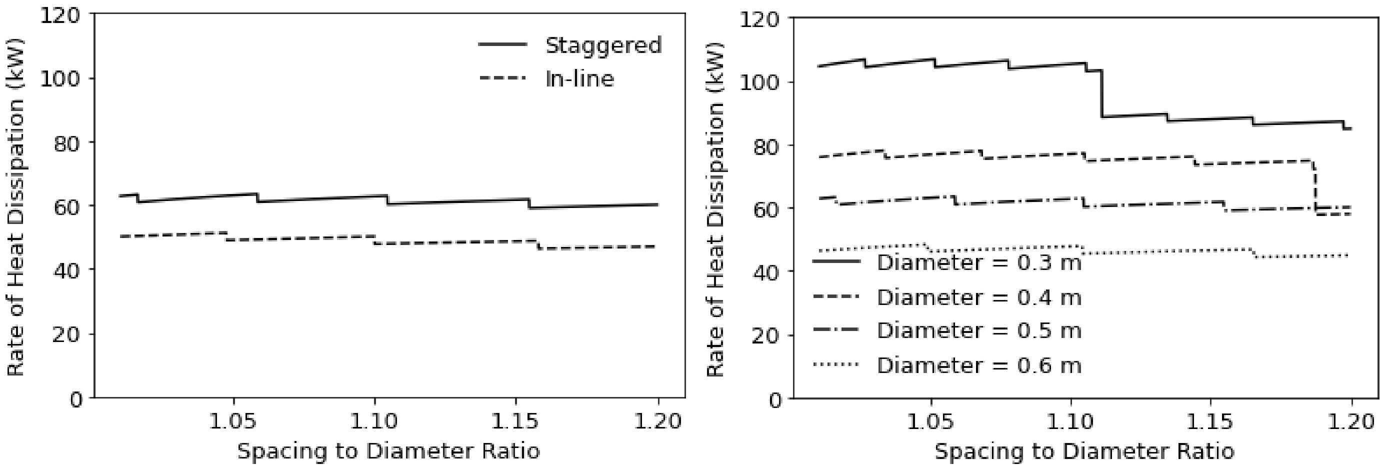
3. Results and Discussion

The model results presented in Fig. 2 show that the heat transfer coefficient for external natural convection in a BGT system is on the order of 2-5 W.m^{-2}.K^{-1}, compared to values upwards of 1000 W.m^{-2}.K^{-1} for internal forced convection during filling of hydrogen cylinders [7]. Therefore the allowable filling rate of a BGT system is limited primarily by the rate of external heat rejection.

The external convective heat transfer coefficient, according to Eq. 11, depends on the temperature difference to the power of 0.27 (Fig. 2b), and on the hydraulic diameter of the channels in between cylinders in proportion to $D_h^{(4\times0.27-1)} = D_h^{0.08}$. Given that heat dissipation is limited primarily by external heat transfer, the overall heat dissipation rate can be maximised (BGT fill time minimised) by injecting hydrogen as rapidly as possible in order to achieve the maximum allowable temperature difference as early as possible in the fill, and then moderating the fill rate to maintain that maximum temperature difference.

The hydraulic diameter depends on the cylinder diameter, cylinder spacing and stagger. Increasing cylinder diameter and spacing both increase D_h, yielding a moderate increase in heat transfer coefficient. Although the in-line cylinder arrangement leaves larger gaps between cylinders than the ‘close-packed’ staggered arrangement, the staggered arrangement increases heat transfer coefficient (Fig 2). However, the total amount of heat dissipated from the system per unit volume of hydrogen stored depends on the cylinder surface area and internal volume as well as the heat transfer coefficient. Therefore, it is necessary to consider also the increase in surface area per unit stored volume offered by reducing cylinder diameter and by use of a staggered arrangement.

A conservative estimate (lower estimate) for the allowable fill rate is given by assuming that all cylinders in the array have the same temperature as the inner cylinder considered in the model set out above. The allowable fill rate is then related to how much heat is dissipated by the inner cylinder and how many such cylinders fit within the container dimensions. The effects of cylinder diameter, spacing and stagger are shown in Figs 3a and b for a system with cylinder surface temperatures of 65℃ and 20℃ ambient temperature. Due to the constraint that cylinders must fit within the container volume, the heat dissipation rate has a discontinuous dependence on cylinder spacing for changes that result in rows or columns of cylinders being removed or added. Despite the lower heat transfer coefficient of smaller diameter cylinders they offer higher surface area per unit volume and hence higher allowable fill rate. The use of a staggered arrangement improves packing density, and the increased surface area and volume both contribute to an increase in allowable fill rate. Increasing cylinder spacing tends to increase heat dissipation, except where it results in cylinders, and the associated surface area and storage volume, being removed from the container.



(a) (b)

Fig. 3 Variations in rate of heat dissipation with spacing to diameter ratio for (a) staggered and in-line arrangements (0.5 m diameter) (b) staggered arrangement with 0.3, 0.4, 0.5, and 0.6 m diameter cylinders.

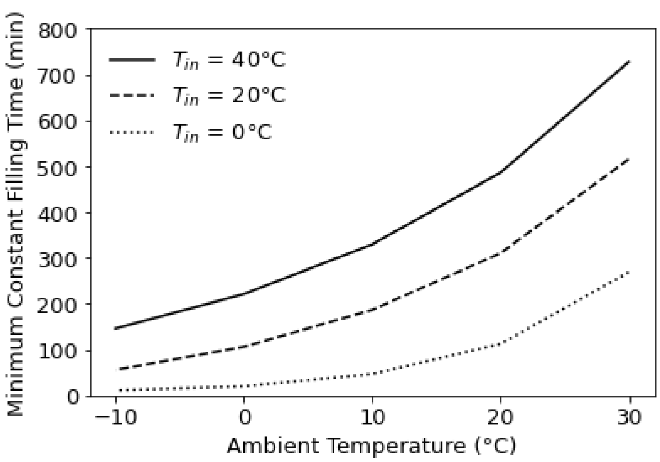


Fig. 4 Variations in the minimum constant filling time of the BGT with ambient temperature and inflow gas temperature.

The cylinder thermal model set out in Section 2 provides simulations of the temperature change during the filling process. In order to illustrate the model's use, Fig. 4 presents fill times for a BGT systems under various environmental and gas supply temperatures. The system comprises 59 cylinders in a staggered arrangement with 0.608 m diameter and 2.338 m length have been simulated between nominal pressures of 20 and 350 barg, setting a temperature limit of 65℃, assuming a constant fill rate. The fill rate has been adjusted iteratively to find the minimum fill time which does not violate the temperature constraint. At 20℃ ambient temperature and 20℃ hydrogen supply, fill times on the order of a few hours are achievable. The fill time increases if the ambient temperature or gas supply temperatures increase, and can be reduced by providing a cooler inflow of hydrogen. Predictions are most sensitive to uncertainty in the modelling of external heat transfer rate, and there is a need for measurement data in order to reduce this uncertainty. The computational simulations provide a valuable tool for investigating design choices, and for understanding and optimising system operation.

4. Conclusions

A low-dimensional model has been developed to provide computationally-inexpensive thermal predictions for the of hydrogen bulk gas transport systems. It is shown that the maximum allowable filling rate is limited by external heat rejection, and modelling is developed to account for natural convective cooling in cylinder arrays. The modelling of external heat transfer has been partially validated and further refined with reference to three-dimensional CFD simulations. The analysis shows that increasing cylinder spacing and cylinder diameter of the cylinders increases heat transfer coefficients, but tends to reduce fill rate on account of reduced surface area within the constrained volume of the BGT container. A staggered arrangement with closely spaced and relatively small diameter cylinders is preferred from the perspective of minimising fill time for a given quantity of hydrogen. The computational model developed provides a valuable design tool for assessing specific design choices and for choosing economically-optimal filling profiles for BGT systems.

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