Optimization of Fast Filling of Hydrogen Cylinders

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Declaration

I, Pau Miquel Mir, declare that this thesis and the work presented in it are my own and has been generated by me as the result of my own original research. I confirm that:

1. This work was done wholly or mainly while in candidature for a degree at this University;
2. Where any part of this thesis has previously been submitted for any other qualification at this University or any other institution, this has been clearly stated;
3. Where I have consulted the published work of others, this is always clearly attributed;
4. Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work;
5. I have acknowledged all main sources of help;
6. Where the thesis is based on work done by myself jointly with others, I have made clear exactly what was done by others and what I have contributed myself;
7. None of this work has been published before submission.

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I also want to thank my parents, for their constant support and for proofreading the paper.

Abstract

This is the abstract.

Contents

Acronyms

CFD Computational Fluid Dynamics

CNG Compressed Natural Gas

FTCS Forward-Time, Centered-Space

ODE Ordinary Differential Equation

PDE Partial Differential Equation

Todo list

1 Introduction

{sec:introduction}

1.1 Purpose of the investigation

Reword

Hydrogen is a very promising alternative fuel for the future, mainly due to the absence of greenhouse emissions when burning it. In this regard, it is superior to petroleum- and, more generally, carbon-based fueling systems currently used by most road vehicles. However, air pollution is a negative externality associated with this type of fuels, as it is a cost to a third party (in this case, society as a whole) that is not accounted for in the price of the good. By definition, the consequences of polluting the air are not included in the price of traditional vehicles, and therefore will have little influence on consumers' choices. Thus, if hydrogen is to succeed as an alternative to carbon-based fuels, it is essential that its use be as convenient, if not more, than traditional fuel.

Cite and include ISO

One of the main aspects where hydrogen currently lags behind traditional fuel is the refueling process. Indeed, refueling hydrogen involves its compression, and thus a significant rise in temperature, which according to standards must be kept below a certain value (358 °K as per SAE J2601). This temperature limit in turn leads to long refueling times, potentially lasting more than five minutes, which is cumbersome for users. Therefore, it is of utmost importance to research and develop systems that enable faster refueling of hydrogen tanks. To this end, this project builds upon a model of filling a hydrogen cylinder which has already been developed by members of the Faculty of Engineering and the Environment at the Univeristy of Southampton to analyse novel methods of improving fill times.

1.2 Outline of the investigation

One of the current solutions to improve fill times involves cooling the hydrogen before filling the cylinder. However, this is quite an expensive process, both in energetic and economic terms. Consequently, the aim of this project is to explore several of the options available to reduce fill times while simultaneously reducing the energy consumption of the process, thus improving both convenience for users and energy efficiency of the fueling stations.

What the fuck are inlet profiles

An attempt to optimise the filling profile of hydrogen cylinders will be made by building upon the existing cylinder model. The model will be developed to include transient effects by implementing a hysteresis effect. This will allow for innovative inlet profiles to be evaluated, such as sinusoidal or square waves . An attempt will be further made to completely determine the ideal filling profile by means of a constrained nonlinear optimization.

2 Background

{sec:background}

2.1 Challenges of hydrogen fuelled for vehicles

{sec:challenges}

Hydrogen is an attractive alternative fuel because it has zero carbon emissions at point of use. In order to exploit hydrogen on road vehicles it is necessary to have practical hydrogen storage and filling infrastructure. Three different technologies have been developed so far: liquid storage systems, metal hydrides, and compressed hydrogen solutions. Liquid storage systems achieve high energy density but require cryogenic cooling solutions, and metal hydrides are an emerging solution that still needs further development to compete with compressed hydrogen. Therefore, this study focuses exclusively on compressed gas storage of hydrogen. To achieve high energy density very high pressures are required, 35 and 70 MPa being the standards. This compressed hydrogen is then used in the fuel cell of the vehicles and converted into electricity, which can be used directly by the electric motor or stored in onboard batteries. The requirements of a compressed hydrogen system are:

- High fuel capacity
- Low overall weight
- Fast fill times

Increasing fuel capacity can be achieved by either using larger tanks, which leads to higher weights, or by using higher pressures. However, fast refueling of hydrogen gas to high pressures leads to a sharp increase in gas temperature due to the Joule-Thompson effect and the quasi-adiabatic compression involved. These higher temperatures are problematic due to material constraints as explained below. This may restrict the fill rate because to avoid exceeding the temperature threshold of the material we may need to allow time for the heat to dissipate through the cylinder walls. Thus, solutions must be developed to minimize the temperature rise when fast filling to high pressures.

yes it gets hot, but how hot is it gonna get. Can prove this by showing temp change with adiabatic filling

Currently, two types of cylinder used are: Type III cylinders, made out of an aluminum liner wrapped in a carbon-fiber/epoxy composite, and Type IV cylinders, with a plastic liner and the same composite wrap. Of concern is the composite material, as the polymer matrix cannot withstand high temperatures, and the material properties of the cylinder will begin to degrade. The specific temperature at which this occurs is usually around the glass transition temperature of the epoxy, where the thermosetting polymer changes from a hard "glassy" state to a more compliant "rubbery" state.

cite: http://www.epotek

2.2 Previous work

This section begins with a summary of previous work concerning heat transfer during fast filling of hydrogen cylinders and concludes with an analysis for the need for more research.

2.2.1 Experimental work

{sec:experimental_w

Several papers describe experimental work that has been conducted regarding the fast-filling of hydrogen cylinders, in particular comparing the results to simulations. Dicken and Mérida's work indicates that the temperature inside the cylinder is rather uniform [1]. This claim is not, however supported by the work of Zheng et al [2] nor that of Woodfield et al [3], wherein large discrepancies among gas temperatures in different regions of the cylinder are found.

2.2.2 Computational Fluid Dynamics (CFD) models

{sec:cfdl

Deal with CFD shit

A large amount of research has been conducted using multidimensional analysis, especially using CFD. Both 2D axisymmetric models and full 3D models have been developed by many authors. 2D models do not include the effects of gravity or buoyancy, but these can be considered negligible. On the other hand, full 3D simulations are computationally expensive and rarely justifiable as the gain in accuracy is very small.

There are many papers describing slightly different methods and setups. The models attempt to solve the Reynolds averaged Navier Stokes equations, which are time averaged equations representing the fluid flow. As these equations are not closed, models for the turbulent viscosity term must be utilised.

Kim et al [4] propose a 3D model with a standard k-ε turbulence model [5] and the Redlich-Kwong real gas equation of state [6] for real gas properties. Dicken and Mérida [7] present an axisymmetric model that uses a modified standard k-ε turbulence model in order to reduce the jet's spreading rate over-prediction of the standard model.

Other investigations use more advanced property models, such as the one presented by Zhao et al [8], which employs REFPROP, a tool developed by the National Institute of Standards and Technology [9], in order to have more precise real gas properties. It uses values of critical and triple points together with equations for the thermodynamic and transport properties to calculate the state points of fluids. Zhao et al's model is validated against experimental results by Zheng et al [2]. In the same spirit, other authors employ more advanced turbulence modelling, such as Heitsch et al's model [10] which uses Menter's Shear Stress Transport turbulence model [11].

Galassi et al [12] present a 3D model using a modified k-ε turbulence model and the Redlich-Kwong real gas equation of state similar to the work by Kim et al [4]. Melideo et al [13] compare an axisymmetric model with this full 3D model and find a very good agreement in the temperature profile, suggesting that the significant extra computation expense of full 3D models might not be necessary. They also use the improved Aungier Redlich Kwang real gas equation of state [14] for improved speed and accuracy.

Most models are built upon existing commercial CFD codes, mainly CFX [**cfx**], used by references [10, 12, 13] and FLUENT [**fluent**], used by references [2, 4, 7, 8].

2.2.3 Zonal models

{sec:zonalModels}

Zonal models, also referred to as a 0-dimensional or reduced order models, consider the gas inside the cylinder as the control volume with homogenous properties. This premise allows for simpler calculations and much lower computational time.

Liu et al [15] assume adiabatic filling of the cylinder. By applying the first law of thermodynamics, they equalled the change in internal energy of the gas to the change in the product of mass and static enthalpy. By then using real gas equations of state, they obtain a simple algebraic equation relating the final temperature in the cylinder to the initial temperature, initial and final pressures.x

Hosseini et al [16] also assume adiabatic filling of the cylinder in addition to a constant mass flow rate in order to simplify the first law of thermodynamics to an Ordinary Differential Equation (ODE). It is solved for internal energy as a function of static enthalpy of the inlet gas, initial specific internal energy, mass flow rate, initial mass, and time. The internal energy can be substituted for a real gas equation to get an expression for temperature as a function of time. not capital

Early work regarding the filling of Compressed Natural Gas (CNG) tanks involves very similar thermodynamics to hydrogen filling. Kountz [17] presented a model which linked an energy balance for the gas to a lumped mass heat conduction model for the cylinder. It used a constant heat transfer coefficient of 28 W/(m^{2}K), although it must be noted that CNG cylinders are filled to lower pressures and during longer fill times.

Woodfield et al [3] coupled a single zone model of the gas in the cylinder with a one dimensional unsteady model for the heat conduction through the cylinder walls. They used the Lee-Kesler method [18] to find the compressibility and thus the density, and from that the mass inside the cylinder.The heat transfer coefficient between the gas and the wall was assumed to 500 W/(m^{2}K) during filling and 250 W/(m^{2}K) after full. double check if true

Similarly, the work by Monde et al [19] uses the same assumption regarding heat transfer coefficient values. They achieve a reasonable fit with experimental data, shown in Fig. 1, even though the measured heat transfer coefficients were significantly lower, as shown in Table 1.

FIGURE 1: Comparison between estimated and measured temperatures by Monde et al [19].

{fig:mondeFit}

P (MPa)		Mass flow rate (g/min)	h (W/(m^{2}K))
5	H_2	168 - 276	86.4 - 97.4
	N_2	456 - 1296	43.0 - 47.0
10	H_2	240 - 324	143.1 - 154.5
	N_2	732 - 996	38.9 - 44.7
35	H_2	45-170	269.7 - 279.2

TABLE 1: Heat transfer coefficients at various conditions by Monde et al [19].

{tab:mondeHValues}

Monde et al [20] used newly published test data to validate their model presented in reference [19]. While the model matches the data reasonably well, different values of heat transfer coefficient have to be employed to achieve a good fit, with recommended values of 150 W/(m^{2}K) and 200 W/(m^{2}K) for filling to 35 MPa and 70 MPa, respectively.

Striednig at al [21] developed a whole-station model linking zero-dimensional models for the storage tank gas, the vehicle tank gas, and the vehicle cylinder. They propose using an annular flow correlation to relate the Nusselt number to the Reynolds number of the flow to dynamically calculate the heat transfer at the wall. However, as they were comparing against data with a Type I cylinder (complete steel construction) they assumed constant temperature through the thickness of the cylinder wall, an assumption which isn't valid for Type III and IV cylinders due to the low thermal conductivity of carbon fiber.

Monde and Woodfield [22] also presented an improved model with a dynamic heat transfer coefficient. The energy balance in the gas is coupled to an unsteady heat conduction equation for the wall. The Nusselt number was derived as a function of Reynolds and Rayleigh numbers by means of an empirical correlation derived from experimental results they presented in reference [23].

A similar model is presented by Johnson et al [24]. While using a proprietary software called Netflow developed by Sandia Labs, a zonal model of the cylinder is created using the same internal energy and mass balance formulation. It considers three different control volumes for the gas: each of the two half domes and the strictly cylindrical section of the tank. Furthermore, it utilizes the Reynolds number of the jet to dynamically calculate the Nusselt number, and thus the heat transfer coefficient, at the wall. The coefficients for these empirical relationships are derived from their experimental results.

cite

Ranong et al [25] present a model with a single zone model for the gas and unsteady heat conduction through the wall. They develop a relationship between Nusselt and Reynolds numbers based upon CFD simulations also presented in that paper. Using this relationship, the heat transfer coefficient is dynamically calculated.

Finally, Khan et al [26] analyzed different tank sizes and optimised fueling characteristics by using the model presented by Monde and Woodfield in references [3, 19, 20]. They use a constant heat transfer coefficient, and make an attempt to evaluate the feasibilty of step-filling. However, the analysis is hindered by the lack of unsteady modelling of the heat transfer coefficient.

2.2.4 Summary and outlook

The simulation work that has been presented in this section, in broad terms, divided into complex CFD models and more simplified reduced dimensional models. It is important to analyze the difference between these two approaches.

Number of degrees of freedom, cells

CFD models have several advantages, as they take into consideration many details that reduced order models must assume, simplify, orneglect. Firstly, one can represent the specific effects of geometry of the cylinder more accurately using CFD. Secondly, time effects can be directly simulated without the need of timescales to be modelled. However, they are extremely computationally expensive, with run times lasting from hours to weeks. It thus follows that the main advantage of reduced dimension models is that they are much less computationally expensive. This, in turn, means they can be incorporated as a part of larger analyses, in which they must be run multiple times, such as optimization routines or probabilistic whole station models.

never mentioned before

In compressed hydrogen fuel systems the gas is at very high pressures, meaning ideal gas approximations are inaccurate, and thus real gas properties must be employed. Several methods are employed in existing work as outlined in Section 2.2.3. Most use real gas equations of state, which although very accurate, are less accurate than property models. Property models determine any gas property from two other independent properties. The property model that will be employed throughout this analysis is REFPROP. Although the use of REFPROP is fairly established in CFD models [2, 8, 24], it is less prominent in reduced order simulations.

Reduced dimension models up to date make assumptions that are not always supported with evidence, and therefore lead to less accurate results. This requires adjustments to the model to match the experimental data, such as the case of Monde et al [20], explained in Section 2.2.3. Although this produces a better fit, the model is less predictive. For this reason, it is important to improve reduced order models by devising ways to obtain quantities previously assumed. This will improve the models' predictive ability, which will increase confidence in results from simulations regarding events which haven't been tried experimentally.

do I have evidence

An assumption typically made is that of a constant heat transfer coefficient derived from either time-averaged experimental results or CFD simulations, as explained in Section 2.2.3. A slightly better assumption employed is that of deriving the heat transfer coefficient from the inlet Reynolds number by means of empirical correlations. However, work conducted so far has used a quasi steady approach to modelling the heat transfer coefficient. This implies either assuming a constant heat transfer coefficient, or deriving it from the instantaneous Reynolds number of the inlet flow. However, for rapid transients, this approach will not work, as the changes in the inflow will inaccurately result in immediate changes to the heat transfer conditions. This report will propose a new method of deriving the unsteady heat transfer coefficient numerically to achieve better results for transient convective heat transfer.

3 Formulation

{sec:formulation}

One of the fundamental principles used throughout this paper, and indeed, throughout engineering, is that of non-dimensioning. By operating using non-dimensional parameters such as the Reynolds number $\mathrm{Re} = \frac{\rho u L}{\nu}$ or the Prandtl number $\mathrm{Pr} = \frac{c_p \mu}{k}$ solving problems involving differential equations becomes simplified. Also, the analysis becomes much more general, and can be scaled.

Out of place, where to put it

3.1 Governing equations

The governing equation for mass and internal energy of the gas in the tank is given by:

$$\frac{dU_{gas}}{dt} = \frac{d\left(m_{gas}u_{gas}\right)}{dt} = h_{in}\dot{m}_{in} - \dot{Q}_{out} \tag{3.1}$$

consistent time derivatives

where U_{gas} is the total internal energy of the gas, m_{gas} is the mass of the gas, u_{gas} is the specific internal energy of the gas, H_in is the enthalpy of the inlet gas, $\dot{m}_{in}$ the mass flow into the cylinder, and $\dot{Q}_{out}$ is the rate of heat transfer out of the gas to the cylinder.

The change in internal energy of the gas is equal to the difference in energy entering the system in the enthalpy of gas inflow and the energy leaving the system through the walls of the cylinder. The enthalpy of the inlet can be determined from real gas models as a function of the inlet pressure and temperature. Therefore, to obtain the internal energy variation one must calculate the gas mass flow and the heat transferred to the cylinder.

We also have conservation of mass in the system, which is expressed simply by:

$$\frac{dm_{gas}}{dt} = \dot{m}_{in} \tag{3.2}$$

as the change in mass of the gas in the cylinder is only influenced by the influx of gas during filling.

One of the simplest methods available to solve this system of ODEs, both conceptually and in terms of ease of implementing in code, is forward Euler time integration. It can be described as follows: given a function that can be defined by:

$$y'(t) = f(t, y(t)), \quad y(t_0) = y_0 \tag{3.3}$$

we can compute the approximate shape of the function given the initial point and finding the slope of the curve for small intervals. Indeed, from the initial point, we can find the tangent of the curve at that point, and take a small step along that tangent until arriving at the next point, where the procedure can be repeated. Denoting the step size as h, we can express forward Euler time integration as:

$$y_{n+1} = y_n + hf(t_n, y_n) \tag{3.4}$$

3.2 Gas mass flow into cylinder

The nozzle and corresponding gas flow will be modeled using isentropic relations, and then a discharge coefficient relationship will be used to find the approximate real values. Indeed, the isentropic Reynold's number is first calculated as follows:

equ:reynoldsIdeal}}

$$\mathrm{Re}_{\text{jet,ideal}} = \frac{\rho_{exit}\, d_{inlet}\, u_{exit}}{\mu_{exit}} \tag{3.5}$$

where d_{inlet} is the diameter of the inlet delivery pipe and ρ_{exit}, u_{exit}, and μ_{exit} are determined using real gas models as described in Section **??**. More specifically:

$$\rho_{exit} = f\left(P_{exit}, S_{in}\right), \quad u_{exit} = \sqrt{2\left(H_{in} - H_{static}\right)}, \quad \mu_{exit} = f\left(P_{exit}, S_{in}\right) \tag{3.6}$$

where P_{exit} is the pressure at the end of the inlet tube, S_{in} is the entropy at the inlet, H_{in} the stagnation enthalpy at the inlet, H_{static} the static enthalpy at the end of the inlet tube, and the function f represents the real gas model which computes a thermodynamic property from any two given properties. As the system is initially treated as isentropic, the inlet entropy can be used to calculate exit properties. We also have:

$$S_{in} = f\left(P_{in}, T_{in}\right), \quad H_{in} = f\left(P_{in}, T_{in}\right), \quad H_{static} = f\left(P_{exit}, S_{in}\right) \tag{3.7}$$

where P_{in} and T_{in} are the inlet pressure and temperature, respectively. The exit pressure P_{exit} is taken to be the pressure inside the gas tank. However, in the case that the inlet diameter is choked, these calculations would yield velocities higher than the speed of sound, which is impossible due to the nature of the inlet pipe. For this reason, if a velocity of Mach 1 or higher is achieved at any given time, an iterative process is used to find the value of P_{exit} that will yield a velocity equal to the speed of sound, and the rest of properties and ultimately the Reynolds number calculated accordingly.

In order to find the real mass flow an empirical discharge coefficient is employed.

$$C_D = \frac{\dot{m}_{in}}{\dot{m}_{ideal}} = c_2 + c_3 \,\mathrm{Re}_{jet,ideal} \tag{3.8}$$

A discharge coefficient must be used to account for the formation of a boundary layer inside the inlet tube. The empirical model that was used was obtained from , and uses the following values: Citation

$$c_2 = 0.938, \quad c_3 = -2.71 \tag{3.9}$$

From the real mass flow the actual Reynold's number of the inflow can be calculated and used to find forced convection heat transfer coefficients in Section 3.3.1 and Eq. (3.14) as follows: avoid forward references

$$\mathrm{Re}_{jet} = \frac{4\dot{m}_{in}}{\pi \mu d} \tag{3.10}$$

3.3 Heat transfer from gas to cylinder

The heat transferred from the gas to the wall of the tank is given by a simple convection relationship:

$$\dot{Q} = hA\left(T_{gas} - T_{wall}\right) \tag{3.11}$$ {{equ:convection}}

where A is the internal surface area of the cylinder, h is the heat transfer coefficient, and T_{gas} and T_{wall} are the temperatures of the gas and the wall, respectively. The heat transfer coefficient is a result of the combination of both forced and natural convection. This is expressed as follows, as per [27] and [28]:

$$h = \sqrt[4]{h_f^4 + h_n^4} \tag{3.12}$$

where h_f is the heat transfer coefficient due to forced convection and h_n is the heat transfer coefficient due to natural convection. Each coefficient can be non-dimensionalised using Nusselt numbers, expressed as:

$$\mathrm{Nu}_f = \frac{h_f D}{k}, \quad \mathrm{Nu}_n = \frac{h_n D}{k} \tag{3.13}$$

where D is the characteristic length, in this case the diameter of the cylinder, and k, the thermal conductivity of the fluid. The values of the Nusselt numbers can be determined from empirical correlations, as detailed in Sections 3.3.1 and 3.3.2.

3.3.1 Forced convection

{sec:forcedConvecti

As the magnitude of heat transfer is related to the flow in forced convection, the Nusselt number can be said to be a function of the Reynolds number, taking the form:

$$\mathrm{Nu}_{f,ss} = c_4 \mathrm{Re}_{jet}^{c_5} \tag{3.14}$$ {{equ:nusseltReyno

where $Nu_{f,ss}$ is the steady state Nusselt number and the empirical constants c_4 and c_5 are given by as:

cite

eltReynoldsConsts}}

$$c_4 =, \quad c_5 = \tag{3.15}$$

The initial work this project builds upon uses the flow at the nozzle to determine the heat transfer at the wall of the cylinder. This assumes that the hydrogen flows instantaneously from the nozzle to the wall, when in reality there is of course a time delay. This assumption is acceptable for stable inflows, hence us referring to the steady state Nusselt number $Nu_{f,ss}$, but for more complex filling patterns and also for improved accuracy it becomes necessary to incorporate hysteresis. Indeed, the heat transfer coefficient at the wall in fact can be said to depend on the nozzle flow seconds prior, or more generally, on the history of the nozzle flow. This can be modeled as follows:

Does this need to be cited / proved? Eplain better so you dont have to cite it

$$\frac{d}{dt}\left(\mathrm{Nu}_f\right) = \frac{\mathrm{Nu}_{f,ss} - \mathrm{Nu}_f}{\tau} \tag{3.16}$$

where τ is the time scale, which reflects the amount of time it takes for the flow to recirculate. Two time scales are considered, as two different situations may be present. The flow in the cylinder may be driven by the inflow of mass from the nozzle, in which case we have a time scale of production τ_{prod}. However, if the inflow halts, the flow field in the cylinder will be driven by the dissipation of the existing flow and thus the time scale is denoted τ_{diss}. Therefore the overall time scale is given by the minimum of these two:

explain why it's minimum

$$\tau = \min\left(\tau_{prod}, \tau_{diss}\right) \tag{3.17}$$

Production time scale The main driver of flow in the cylinder, which in turn drives convective heat transfer, is the turbulent jet that develops from the end of the nozzle throughout the length of the cylinder. Experimental results can be used to derive expressions for the axial velocity of the jet. Radial profiles of mean axial velocity can be seen in Fig. 2.

FIGURE 2: Radial profiles of mean axial velocity in a turbulent round jet with Re = 95,000. Adapted from [29] with the data from [30]

{fig:radialProfile}

By plotting the inverse of the non-dimensional speed, $u_{exit}/u(x)$ against x/d we get the clearly linear relationship shown in Fig. 3.

FIGURE 3: Jet speed vs distance. Adapted from [29] with the data from [30]

{fig:jetSpeed}

From this experimental result the following relationship is obtained:

{{equ:axialSpeed}}

$$\frac{u(x)}{u_{exit}} = \frac{c_1}{(x - x_0)/d_{inlet}} \tag{3.18}$$

where $u(x)$ is the axial velocity at a distance x from the nozzle, x_0 is the position of the virtual origin, and c_1 is an empirical constant.

The production time scale is given by the spatial integral of the axial speed of the jet, which is given in Eq. (3.18) in **??**.

$$\begin{aligned}\tau_{prod} &= \int_0^L \frac{1}{u(x)}dx = \frac{1}{c_1 u_{exit}} \int_0^L (x - x_0)\,dx \\ &= \frac{\frac{L^2}{2} - x_0 L}{c_1 u_{exit} d}\end{aligned} \tag{3.19}$$

As we have $x_0 \ll L$ we can write:

$$\tau_{prod} = \frac{L^2}{2c_1 u_{exit} d} \tag{3.20}$$

and defining $c_6 = \frac{1}{2c_1}$:

$$\tau_{prod} = c_6 \frac{L^2}{u_{exit} d} \tag{3.21}$$

Dissipation time scale The dissipation time scale can be said to be proportional to the length of the cylinder L and the recirculation velocity u_{recirc}: need to explain why?

$$\tau_{diss} = c_7 \frac{L}{u_{recirc}} \tag{3.22}$$

We can then define the Reynolds number of the recirculation flow as:

$$\mathrm{Re}_{recirc} = \frac{u_{recirc} D}{\nu} \tag{3.23}$$

Let us assume that instantaneous Nusselt number depends on u_{recirc} as it depends on Re^{c_5} and $c_5 \sim \mathcal{O}(1)$. From Eq. (3.14) we know that:

$$\frac{D u_{recirc}}{\nu} = c_8 \mathrm{Nu}_f \tag{3.24}$$

We can therefore rewrite:

$$\tau_{diss} = \frac{c_7}{c_8} \frac{LD}{\nu \mathrm{Nu}_f} \tag{3.25}$$

Combining the two constants and absorbing the L/D coefficient:

$$\tau_{diss} = c_9 \frac{L^2}{\nu \mathrm{Nu}_f} \tag{3.26}$$

We can then make use of the fact that in steady state we know $\tau_{prod} = \tau_{diss}$, which leads to:

$$c_9 \frac{L^2}{\nu \mathrm{Nu}_f} = c_6 \frac{L^2}{u_{exit} d} \tag{3.27}$$

Substituting the definitions of Nusselt and Reynolds numbers from Eqs. (3.5) and (3.14):

$$c_9 = c_6 \frac{\nu \mathrm{Nu}_f}{u_{exit} d} = c_4 c_6 \tag{3.28}$$

Which leads to a final definition of τ_{diss} in terms of literature constants:

$$\tau_{diss} = \frac{c_4}{2c_1} \frac{L^2}{\nu \mathrm{Nu}_f} \tag{3.29}$$

Therefore, in a pure dissipation scenario, where $\mathrm{Nu}_{f,ss} \to 0$, we have:

$$\frac{d}{dt}\left(\mathrm{Nu}_f\right) = -\mathrm{Nu}_f^2 \frac{2c_1}{c_4} \frac{\nu}{L^2} \tag{3.30}$$

which can be solved by simple integration, which yields:

$$\int_{Nu_{initial}}^{Nu(t)} -\frac{dNu_f}{Nu_f^2} = \int_0^t \frac{2c_1}{c_4} \frac{\nu}{L^2} dt \tag{3.31}$$

$$Nu_f = \frac{c_4}{2c_1} \frac{L^2}{\nu} \frac{1}{t} \tag{3.32}$$

3.3.2 Natural convection

:naturalConvection}

Natural convection is caused by buoyancy driven flow, so the natural Nusselt number can be found to be related to the Rayleigh's number (itself a product of Grashof's and Prandt's numbers) by the following relationship:

$$\mathrm{Nu}_n = c_{10} \mathrm{Ra}^{c_{11}} \tag{3.33}$$

where Rayleigh's number is defined as:

$$\mathrm{Ra} = \left| \frac{g\beta \left(T_{wall} - T_{gas}\right) D^3}{\nu \alpha} \right| \tag{3.34}$$

where g is the acceleration due to gravity, β is the coefficient of thermal expansion, D is the characteristic length, in this case the cylinder diameter, ν is the kinematic viscosity, and α is the thermal diffusivity, as defined by:

ermalDiffusivity}}

$$\alpha = \frac{k}{\rho c} \tag{3.35}$$

where k is the material's thermal conductivity, ρ is the density of the material, and c is the specific heat capacity of the material. The coefficients are given by :

cite

$$c_{10} =, \quad c_{11} = \tag{3.36}$$

FIGURE 4: Diagram show composition of wall and heat fluxes into and out of wall.

{fig:wall}

3.4 Heat transfer across cylinder

The main mode of heat transfer that occurs in the cylinder and that will be used throughout this report is heat conduction through the wall of the cylinder. A diagram showing the heat transfer through the wall is shown in Fig. 4. The heat transfer is modeled using one dimensional unsteady heat conduction:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \tag{3.37}$$ {{equ:heatEquation}

where α is the thermal diffusivity, as defined in Eq. (3.35). The boundary condition at the inner wall can be described by equalling the heat flux into the wall from convection to the conduction through the wall:

$$k \frac{dT_w}{dx}\bigg|_{x=0} = hA\left(T_{gas} - T_{wall}\right) \tag{3.38}$$ {{equ:innerWallBC}}

For the boundary between the liner and the laminate a point precisely on the boundary is considered. At that point, the heat flux through the liner material and the heat flux through the laminate material and the respective temperatures must be equal:

$$\begin{gathered} k_{lin} \frac{\partial T_{lin}}{\partial x} = k_{lam} \frac{\partial T_{lam}}{\partial x} \\ T_{lin} = T_{lam} \end{gathered} \tag{3.39}$$

Solving this equation will yield the temperature distribution throughout the thickness of the cylinder wall, and more specifically, the internal wall temperature that is used to calculate the heat transferred out of the gas in Eq. (3.11).

3.4.1 Outer Wall

Several cases can be considered for the outer wall, and the investigations described in Section 2.2.3 employ different boundary conditions. A constant heat flux can be applied to the outer wall, be it a constant heat loss or an adiabatic condition. The adiabatic condition represents the situation in which the cylinders are in an enclosed space which cannot transfer heat to the environment efficiently enough for it to affect he temperature of the tanks. this is the most conservative approach. Having a constant heat loss can be somewhat of an oversimplification, but a natural convection relationship could be employed to represent the heat loss to the environment in a more open environment. However, the approach used in this report will be the adiabatic condition, which can be expressed as follows:

$$\frac{\partial T_C}{\partial x} = 0 \tag{3.40}$$

where T_C is the outer wall temperature.

3.4.2 Discretisation

In order to solve the heat equation Partial Differential Equation (PDE) presented in Eq. (3.37) a discretisation method must be employed. The scheme employed is known as Forward-Time, Centered-Space (FTCS), first described as such by Roache [31].

$$\frac{T_{i+1,j}-T_{i,j}}{\Delta t}=\alpha\frac{T_{i,j+1}-2T_{i,j}+T_{i,j-1}}{\Delta x^2} \tag{3.41}$$

where the i and j subscripts represent the nodes of the discretisation in time and space, respectively, Δt is the time step, and Δx is the distance between grid points. This can be rearanged for $T_{i+1,j}$ and substituting $r=\frac{\alpha\Delta t}{\Delta x^2}$, we have:

$$T_{i+1,j}=T_{i,j}+r\left(T_{i,j+1}-2T_{i,j}+T_{i,j-1}\right) \tag{3.42}$$

The scheme is numerically stable if and only if [32]:

$$r=\frac{\alpha\Delta t}{\Delta x^2}<\frac{1}{2} \tag{3.43}$$

We can also apply the discretisation scheme on the boundary conditions. For the inner wall boundary condition expressed in Eq. (3.38) we can write:

finish

$$T_{i+1,j}=T_{i,j}+2r\left(T_{i,j+1}-T_{i,j}+\frac{\Delta x\, h\left(T_{gas}-T_{i,j}\right)}{k_{lin}}\right) \tag{3.44}$$

$$T_{i+1,j}=T_{i,j}+\frac{\Delta t}{\Delta x^2}\left(\frac{k_{lam}\left(T_{i,j+1}-T_{i,j}\right)-k_{lin}\left(T_{i,j}-T_{i,j-1}\right)}{0.5\left(C_{lin}\rho_{lin}+C_{lam}\rho_{lam}\right)}\right) \tag{3.45}$$

3.5 Throttling

Throttling is introduced in order to more accurately represent real life conditions. When a maximum temperature is reached, the inflow of hydrogen must be stopped in order to protect the materials of the tank, as detailed in Section 2.1. A simple method of throttling, with the flow stopping at the designated maximum temperature, 85 °C, and the flow restarting at a chosen temperature. The optimum temperature at which flow restarts was considered in this study, and results are presented in **??**

3.6 Optimization

The optimization was realized using a constrained nonlinear multivariable minimiser. It accepts problems in the following form:

$$min f(x) \text{ such that } \begin{cases} c(x) & \leq 0 \\ ceq(x) & = 0 \\ A \cdot x & \leq b \\ Aeq \cdot x & = beq \\ lb \leq x & \leq ub \end{cases} \tag{3.46}$$

where x is the input variable; A and Aeq, and b and beq are matrices and vectors respectively which describe the linear constraints, $c(x)$ and $ceq(x)$ are nonlinear functions constraining x, and lb and ub are vectors which describe the upper and lower bounds of the problem [**fmincon**].

The optimization problem for the hydrogen filling can be expressed as follows:

$$min f(x) \text{ such that } c(x) \leq 85 \tag{3.47}$$

where $f(x)$ returns the fill time given inlet pressure profile parameters x, and $c(x)$ returns the maximum temperature reached by the gas inside the cylinder during the duration of the fill. The parameters x described can create several profiles:

- $x = m$, $P(t) = mt + P_0$
- $x = [A, B, C]$, $P(t) = A \cdot \sin\left(\frac{2\pi}{B}t\right) + Ct$
- $x = [A, B, C, D]$, $P(t) = A \cdot g\left(\frac{2\pi}{B}t, C\right) + Dt$, where $g(x, d)$ creates a square wave with duty cycle d.
- $x = [P_1, P_2, ..., P_n]$, $P(t) = h(P_1, P_2, ..., P_n)$ where $h([P])$ is a spline interpolating function.

By specifying which type profile will be used, the optimiser will take the initial parameters, find the fill time and maximum temperature, and use finite differences to find the partial derivatives $\frac{\partial f}{\partial x_i}$ and $\frac{\partial c}{\partial x_i}$. From there, the interior point algorithm [**interiorPoint**] will choose a new set of parameters, and repeat the process. This will continue until the first order optimality, that is, a measure of how close to a local minimum the objective function is [**firstOrderOpt**], reaches a given threshold.

General stuff:
- Check tense and person
- Check for repetition
- Check for excessive verboseness - define short and long cylinders at some point

4 Results and Discussion
{sec:results}

4.1 Fitting to CFD data

4.2 Square wave inlet profile

4.3 Random inlet profile

5 Conclusion
{sec:conclusion}

This is the conclusion.

Appendices

A Filling Code

{app:filling_code}

```
function [x,f,eflag,outpt] = provaOpt(x0, profileFunction, lb, ub)

options = optimoptions('fmincon','Display','iter-detailed','Algorithm',...
                       'interior-point','UseParallel',true,'Diagnostics',...
                       'on', 'OutputFcn', @outfun);


% Set up shared variables with OUTFUN
history.x = [];
history.fval = [];
searchdir = [];


xLast = []; % Last place computeall was called
myf = []; % Use for objective at xLast
myc = []; % Use for nonlinear inequality constraint
myceq = []; % Use for nonlinear equality constraint

fun = @objfun; % the objective function, nested below
cfun = @constr; % the constraint function, nested below

A = [];
b = [];
Aeq = [];
beq = [];

% Call fmincon
[x,f,eflag,outpt] = fmincon(fun,x0,A,b,Aeq,beq,lb,ub,cfun,options);

    function y = objfun(x)
        sprintf('X = %2.16e   ', x)
        if ~isequal(x,xLast) % Check if computation is necessary
            disp("Evaluating objective function")
            [myf,myc,myceq] = MainRoutine(x, profileFunction);
            xLast = x;
        else
            disp("Obtaining evaluated objective function")
        end
        % Now compute objective function
        y = myf;
    end

    function [c,ceq] = constr(x)
        sprintf('X = %2.16e   ', x)
        if ~isequal(x,xLast) % Check if computation is necessary
            disp("Evaluating nonlinear constraints")
            [myf,myc,myceq] = MainRoutine(x, profileFunction);
            xLast = x;
        else
            disp("Obtaining evaluated nonlinear constraints")
        end
        % Now compute constraint functions
        c = myc; % In this case, the computation is trivial
        ceq = myceq;
    end

    function stop = outfun(x,optimValues,state)
    stop = false;

       switch state
           case 'init'
```

```
                hold on
            case 'iter'
                % Concatenate current point and objective function
                % value with history. x must be a row vector.
                history.fval = [history.fval; optimValues.fval];
                history.x = [history.x; x];
                % Concatenate current search direction with
                % searchdir.
                searchdir = [searchdir;...
                             optimValues.searchdirection'];

                plot(x(1),x(2),'o');
                % Label points with iteration number.
                % Add .15 to x(1) to separate label from plotted 'o'
                text(x(1)+.15,x(2),num2str(optimValues.iteration));

                plot(profileFunction(x, 2000),)

            case 'done'
                hold off
            otherwise
        end
    end

end
```

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