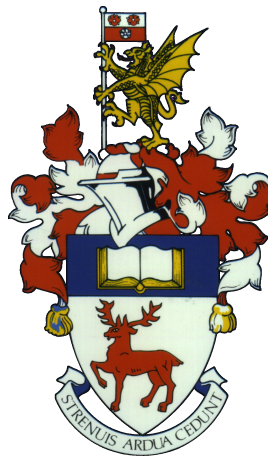


1 **Novel Approaches to Fast Filling of Hydrogen Cylinders**

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4 This report is submitted in partial fulfillment of the requirements for the MEng Mechanical
5 Engineering, Faculty of Engineering and the Environment, University of Southampton.

6

Declaration

7

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:

8

9

1. This work was done wholly or mainly while in candidature for a degree at this University;

10

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;

11

12

3. Where I have consulted the published work of others, this is always clearly attributed;

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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;

14

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5. I have acknowledged all main sources of help;

16

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;

17

18

7. None of this work has been published before submission.

19

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20

I want to thank my advisor, Dr. Edward Richardson, for his time, dedication, patience, and support throughout this project.

21

22

Furthermore, I would like to thank Vishagen Ramasamy for his initial work upon which this paper builds.

23

24

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25

Abstract

26

This is the abstract.

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59 **References**

19

60 **Acronyms**

61 **CFD** Computational Fluid Dynamics

62 **FTCS** Forward-Time, Centered-Space

63 **ODE** Ordinary Differential Equation

64 **PDE** Partial Differential Equation

65 **Todo list**

66	Reword	1
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68	reword this crap	1
69	yes it gets hot, but how hot is it gonna get. Can prove this by showing temp change with	
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71	cite: http://www.epotek.com/site/files/Techtips/pdfs/tip23.pdf	2
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80	cite	8
81	Does this need to be cited / proved? Eplain better so you dont have to cite it	8
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86	- Check tense and person	
87	- Check for repetition	
88	- Check for excessive verboseness - define short and long cylinders at some point . . .	12

1 Introduction

1.1 Purpose of the investigation

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 current petroleum- and, more generally, carbon-based fueling systems currently used by most road vehicles. However, air pollution is a negative externality associated with carbon-based 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 negative consequences of polluting the air are not accounted for in the price of carbon vehicles, and therefore will have little influence on a consumer's choice. Thus, if hydrogen is to succeed as an alternative to carbon fuels, it is essential that its use be as, if not more, convenient than traditional fuel.

One of the main aspects where hydrogen currently lags behind traditional fuel is the refueling experience. Given that refueling hydrogen involves its compression, there is a significant rise in temperature, which must be kept below certain standards (358 °K as per SAE J2601). This in turn leads to long refueling times, potentially lasting more than five minutes, which is cumbersome for users. Therefore, it is of prime importance to research and develop systems that enable faster refueling of hydrogen cylinders. To this end, this project builds upon a model of filling a hydrogen cylinder which has already been developed by members of the department 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 as to keep it below the maximum temperature. However, this is quite expensive, both in energy terms and in economic terms. Consequently, the aim of this project is to continue exploring several of the options available to reduce fill times and simultaneously reduce the energy consumption of the process, thus improving both convenience for users and energy efficiency of the fueling stations. Indeed, by building upon the existing cylinder model several options shall be considered, namely: refrigeration, flow regulation, heat sink usage, active cooling, heat pipe usage, and phase change materials. From here, several options are open to further deepen or potentially broaden the investigation. An attempt to further simplify the model can be made, perhaps even reducing it to a simple algebraic relationship. Also, the model would benefit from FEA validation to aid our understanding of the heat transfer in the structure. This would go hand in hand with analysing the temperature of the structure, and seeing how close this matches the gas temperature. Indeed, if the structure is at a much lower temperature than the gas, the case can be made that the current regulations are slightly erroneous, as they are meant to protect the materials of the structure, but instead regulate the gas temperature.

2 Background

2.1 Challenges for compressed hydrogen storage 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. Using liquid storage systems achieves high energy density but requires cryogenic cooling solutions. Metal hydrides are an emerging solution that still needs further development to compete with compressed hydrogen. This study focuses exclusively on compressed gas storage of hydrogen. In order to achieve high energy density very high pressures are required, 35 and 70 MPa being the standards. This hydrogen is then used in the fuel cell 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

These goals have certain implications. First, it is clear that several tradeoffs and compromises must be made. Increasing fuel capacity can be done by either using larger tanks, which leads to higher weight, or using higher pressures. However, fast refueling of hydrogen gas to high pressures leads to a sharp increase in 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 in order 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.

Currently, the two main 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 as such 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.

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

cite:
<http://www.epotek.com>

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.

157 2.2.1 Experimental work

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

163 2.2.2 Modeling Work

164 **Computational Fluid Dynamics (CFD)** A large amount of research has been conducted using
 165 multidimensional analysis, especially using CFD. Both 2D axisymmetric models and full 3D models
 166 have been developed by many authors. 2D models will not include the effects of gravity or buoyancy,
 167 but these can be considered negligible, and the computational expense of full 3D simulations is rarely
 168 justifiable as the gains in accuracy are very small.

169 There are many papers describing different methods and setups, such as Dicken and Mérida's
 170 work, which uses the standard k- ϵ turbulence model and the Redlich-Kwong real gas equation of
 171 state for real gas properties [4]. Other investigations use more advanced property models, such as
 172 the one presented by Zhao et al., which employs REFPROP (see Section 2.3.2) in order to have more
 173 precise real gas properties [5].

174 **Zonal model** Less work has been conducted regarding zonal models. A zonal model, also re-
 175 ferred to as a 0-dimensional or reduced order model, considers the gas inside the cylinder as the
 176 control volume, with homogenous properties. This allows for simpler calculations and much lower
 177 computational time.

178 Woodfield et al [3] coupled a single zone model of the gas in the cylinder with a one dimensional
 179 unsteady model for the heat conduction through the cylinder walls. They used the Lee-Kesler method
 180 [6] to find the compressibility and thus the density and from that the mass inside the cylinder. The
 181 heat transfer coefficient between the gas and the wall was assumed to be constant: 500 W/(m²K)
 182 during filling and 250 W/(m²K) after full.

183 Similarly, the work by Monde et al [7] uses the same assumption regarding heat transfer coeffi-
 184 cient values. They achieve a reasonable fit with experimental data, shown in Fig. 1, even though the
 185 measured heat transfer coefficients were significantly lower, shown in Table 1.

FIGURE 1: Comparison between estimated and measured temperatures by Monde et al [7]

{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 [7]

A similar model is presented by Johnson et al [8]. 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 Reynold's number of the jet to dynamically calculated the Nusselt's number, and thus the heat transfer coefficient, at the wall

cite

2.2.3 Analysis

The simulation work that has been conducted can be, in broad terms, divided into complex CFD models and more simplified reduced dimensional models. It is important to analyze the difference between these two systems.

CFD models have several advantages, as they take into consideration many things which reduced order models must simplify, neglect or assume. 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

Reduced dimension models up to date make assumptions that are difficult to support with evidence, and therefore lead to results not being very accurate. This leads to adjustments being made to the model to match the experimental data from the same experiment, which produces a better fit for the model, but leads to a less predictive model. For this reason, it is important to improve reduced order models by devising ways to calculate 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

For instance, they assume a homogenous gas temperature, which, as outlined in Section 2.2.1, is supported by some experimental work, but refuted by others. For this reason, more research should be conducted to validate the uniform gas temperature approximation. Another assumption typically made is a constant heat transfer coefficient derived from time-averaged experimental results, as explained in Section 2.2.2. This report will propose a new method of deriving the heat transfer

who is they

coefficient numerically to achieve better results.

2.3 Methodology

Several techniques and methods will be used throughout the analysis. These are described in this section.

2.3.1 Non-dimensioning

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 $Re = \frac{\rho u L}{\mu}$ or the Prandtl number $Pr = \frac{c_p \mu}{k}$ solving problems involving differential equations becomes simplified. Also, the analysis becomes much more general, and can be scaled.

2.3.2 Numerical methods

Integrating Ordinary Differential Equations (ODEs) A central part of solving unsteady heat transfer problems involves integrating ODEs, as will be seen in Section 3. One of the simplest methods available, 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:

$$y'(t) = f(t, y(t)), \quad y(t_0) = y_0 \quad (2.1)$$

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:

$$y_{n+1} = y_n + hf(t_n, y_n) \quad (2.2)$$

Property models As the gases that are being treated in this report are at very high pressures, ideal gas approximations are inaccurate, and thus real gas properties must be employed. To this end, property models must be used, which can determine any gas property from two other independent properties.

The property model that will be employed throughout this analysis is REFPROP, a tool developed by the National Institute of Standards and Technology [9]. It uses values of critical and triple points together with equations for the thermodynamic and transport properties to calculate the state points of fluids.

3 Formulation

3.1 Governing equations

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

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

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:

$$\frac{dm_{gas}}{dt} = \dot{m}_{in} \quad (3.2)$$

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

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:

$$\text{Re}_{ideal} = \frac{\rho_{exit} d_{inlet} u_{exit}}{\mu_{exit}} \quad (3.3) \quad \{\text{equ:reynoldsIdeal}\}$$

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 2.3.2. More specifically:

$$\rho_{exit} = f(P_{exit}, S_{in}), \quad u_{exit} = \sqrt{2(H_{in} - H_{static})}, \quad \mu_{exit} = f(P_{exit}, S_{in}) \quad (3.4)$$

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. As the system is treated as isentropic, the inlet entropy can be used to calculate exit properties. We also have:

$$S_{in} = f(P_{in}, T_{in}), \quad H_{in} = f(P_{in}, T_{in}), \quad H_{static} = f(P_{exit}, S_{in}) \quad (3.5)$$

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.

$$C_D = \frac{\dot{m}_{in}}{\dot{m}_{ideal}} = c_2 + c_3 \text{Re}_{ideal} \quad (3.6)$$

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 [10], and uses the following values:

$$c_2 = 0.938, \quad c_3 = -2.71 \quad (3.7)$$

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. (3.12) as follows:

$$\text{Re} = \frac{4\dot{m}_{in}}{\pi\mu d} \quad (3.8)$$

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:

$$\dot{Q} = hA(T_{gas} - T_{wall}) \quad (3.9)$$

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 [10] and [11]:

$$h = \sqrt[4]{h_f^4 + h_n^4} \quad (3.10)$$

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's numbers, expressed as:

$$\text{Nu}_f = \frac{h_f D}{k}, \quad \text{Nu}_n = \frac{h_n D}{k} \quad (3.11)$$

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's numbers can be determined from empirical correlations, as detailed in Sections 3.3.1 and 3.3.2.

3.3.1 Forced convection

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

$$Nu_{f,ss} = c_4 Re^{c_5} \quad (3.12) \quad \{\text{equ:nusseltReynol}\}$$

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

$$c_4 = , \quad c_5 = \quad (3.13) \quad \{\text{equ:nusseltReynol}\}$$

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's 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:

$$\frac{d}{dt}(Nu_f) = \frac{Nu_{f,ss} - Nu_f}{\tau} \quad (3.14)$$

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:

$$\tau = \min(\tau_{prod}, \tau_{diss}) \quad (3.15)$$

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 [12] with the data from [13]

{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 [12] with the data from [13]

{fig:jetSpeed}

312 From this experimental result the following relationship is obtained:

$$\frac{u(x)}{u_{exit}} = \frac{c_1}{(x - x_0)/d_{inlet}} \quad (3.16) \quad \{\text{equ:ax}\}$$

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

315 The production time scale is given by the spatial integral of the axial speed of the jet, which is
316 given in Eq. (3.16) in ??.

$$\begin{aligned} \tau_{prod} &= \int_0^L \frac{1}{u(x)} dx = \frac{1}{c_1 u_{exit}} \int_0^L (x - x_0) dx \\ &= \frac{\frac{L^2}{2} - x_0 L}{c_1 u_{exit}} \end{aligned} \quad (3.17)$$

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

$$\tau_{prod} = \frac{L^2}{2c_1 u_{exit}} \quad (3.18)$$

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

$$\tau_{prod} = c_6 \frac{L^2}{u_{exit} d} \quad (3.19)$$

319 **Dissipation time scale** The dissipation time scale can be said to be proportional to the length of
320 the cylinder L and the recirculation velocity u_{recirc} :

$$\tau_{diss} = c_7 \frac{L}{u_{recirc}} \quad (3.20)$$

321 Let us assume that instantaneous Nusselt's number depends on u_{recirc} as it depends on Re^{c_5} and
322 $c_5 \sim \mathcal{O}(1)$. From Eq. (3.12) we know that:

$$\frac{Du_{recirc}}{\nu} = c_8 Nu_f \quad (3.21)$$

323 We can therefore rewrite:

$$\tau_{diss} = \frac{c_7}{c_8} \frac{LD}{\nu Nu_f} \quad (3.22)$$

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

$$\tau_{diss} = c_9 \frac{L^2}{\nu Nu_f} \quad (3.23)$$

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

need to explain
why?

$$\tau_{diss} = c_9 \frac{L^2}{\nu \text{Nu}_f} = c_6 \frac{L^2}{u_{exit} d} \quad (3.24)$$

326 Substituting the definitions of Nusselt's and Reynolds numbers from Eqs. (3.3) and (3.12):

$$c_9 = c_6 \frac{\nu \text{Nu}_f}{u_{exit} d} = c_4 c_6 \quad (3.25)$$

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

$$\tau_{diss} = \frac{c_4}{2c_1} \frac{L^2}{\nu \text{Nu}_f} \quad (3.26)$$

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

$$\frac{d}{dt} (\text{Nu}_f) = -\text{Nu}_f^2 \frac{2c_1}{c_4} \frac{\nu}{L^2} \quad (3.27)$$

329 which can be solved by simple integration, which yields:

$$\int -\frac{d\text{Nu}_f}{\text{Nu}_f^2} = \int \frac{2c_1}{c_4} \frac{\nu}{L^2} dt \quad (3.28)$$

$$\text{Nu}_f = \frac{c_4}{2c_1} \frac{L^2}{\nu} \frac{1}{t} \quad (3.29)$$

330 3.3.2 Natural convection

{sec:naturalConvection}

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

$$\text{Nu}_n = c_{10} \text{Ra}^{c_{11}} \quad (3.30)$$

334 where Rayleigh's number is defined as:

$$\text{Ra} = \left| \frac{g\beta (T_{wall} - T_{gas}) D^3}{\nu \alpha} \right| \quad (3.31)$$

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

$$\alpha = \frac{k}{\rho c} \quad (3.32) \quad \{\text{equ:thermalDiffusivity}\}$$

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

cite

$$c_{10} =, \quad c_{11} = \quad (3.33)$$

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. This is modeled using:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad (3.34)$$

where α is the thermal diffusivity, as defined in Eq. (3.32). 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:

$$k \frac{dT_w}{dx} \Big|_{x=0} = hA (T_{gas} - T_{wall}) \quad (3.35)$$

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. (3.9).

3.4.1 Outer Wall

3.4.2 Discretisation

In order to solve the heat equation Partial Differential Equation (PDE) presented in Eq. (3.34) a discretisation method must be employed. The scheme employed is known as Forward-Time, Centered-Space (FTCS).

$$\frac{T_{i+1,j} - T_{i,j}}{\Delta t} = \alpha \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{\Delta x^2} \quad (3.36)$$

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 rearranged for $T_{i+1,j}$ and substituting $r = \frac{\alpha \Delta t}{\Delta x^2}$, we have:

$$T_{i+1,j} = T_{i,j} + r(T_{i,j+1} - 2T_{i,j} + T_{i,j-1}) \quad (3.37)$$

We can also apply the discretisation scheme on the boundary conditions. For the inner wall boundary condition expressed in Eq. (3.35) we can write:

$$T_{i+1,j} = T_{i,j} + 2r \left(T_{i,j+1} - T_{i,j} + \frac{\Delta x h (T_{gas} - T_{i,j})}{k_{lin}} \right) \quad (3.38)$$

$$T_{i+1,j} = T_{i,j} + \frac{\Delta t}{\Delta x^2} \left(\frac{k_{lam} (T_{i,j+1} - T_{i,j}) - k_{lin} (T_{i,j} - T_{i,j-1})}{0.5 (C_{lin} \rho_{lin} + C_{lam} \rho_{lam})} \right) \quad (3.39)$$

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

General stuff:

- Check tense and person
- Check for repetition
- Check for excessive verbosity - define short and long cylinders at some point

³⁶⁸ 4 Results and Discussion

{sec:results}

³⁶⁹ 5 Conclusion

{sec:conclusion}

³⁷⁰ This is the conclusion.

371 **Appendices**372 **A Filling Code**

{app:filling_code}

```

1  %Author: Vishagen Ramasamy
2  %Date: -
3
4  % Copyright University of Southampton 2017.
5  % No warranty either expressed or implied is given to the results produced
6  % by this software. Neither the University, students or its employees
7  % accept any responsibility for use of or reliance on results produced by
8  % this software.
9
10 %% script that computes the filling of the tank(s)
11 %% Importing the pressure and temperature profile at the entrance of the delivery pipe from Dicken and Merida
12 % and calculating the stagnation enthalpy and entropy
13
14 for j = 1:maxt
15     time(j+1) = (j)*dt; % Time as filling proceeds
16     for i = 1:tank_number
17         % Select inlet pressure / temperature profile based on user input
18         if blnUseStandardData == 1
19             % Constant inlet pressure profile
20             P_inlet(i,j+1) = ConstPressKPa;
21         else
22             % Read inlet pressure profile from specified file
23             P_inlet(i, j+1) = interp1(InletPressureData(:,1),InletPressureData(:,3), dt*j);
24         end
25
26         if blnUseStandardData == 1
27             %Temp_inlet(i,j+1) = interp1(time_in, temp_in, dt*j); % Temperature profile after the first 1.35 s
28             Temp_inlet(i, j+1) = ConstTempK;
29         else
30             % Read inlet temperature profile from specified file
31             Temp_inlet(i, j+1) = interp1(InletTempData(:,1), InletTempData(:,3), dt*j);
32         end
33
34         h_inlet(i,j+1) = refpropm('H','T',Temp_inlet(i,j+1),'P',P_inlet(i,j+1),Fluid{i}, refpropdir); % R
35         entropy_inlet(i,j+1) = refpropm('S','T',Temp_inlet(i,j+1),'P',P_inlet(i,j+1),Fluid{i}, refpropdir); % R
36
37         %% Determine which pressure to use at the exit of the delivery pipe which is dependent upon the number o
38
39         if l_d(i) > 3 && blnOneZone{i} == 0 % The length-to-diameter ratio of the tank(s) determines th
40             Pressure_exit = P_gas_zone1{i}(j); % The pressure at the exit of the delivery pipe is equal to the
41         else
42             Pressure_exit = P_gas(i,j); % The pressure at the exit of the delivery pipe is equal to the
43         end
44
45         if (P_inlet(i,j+1) > Pressure_exit) % condition for filling of tank(s)
46             sound_exit(i,j+1) = refpropm('A','P',Pressure_exit,'S',entropy_inlet(i,j+1),Fluid{i}, refpropdir);
47             h_static_exit(i,j+1) = refpropm('H','P',Pressure_exit,'S',entropy_inlet(i,j+1),Fluid{i}, refpropdir);
48             visc_exit(i,j+1) = refpropm('V','P',Pressure_exit,'S',entropy_inlet(i,j+1),Fluid{i}, refpropdir);
49             mach_exit(i,j+1) = sqrt(2*(h_inlet(i,j+1)-h_static_exit(i,j+1))/sound_exit(i,j+1)^2); % Calculates
50
51             %% If Mach number is greater than one, the exit pressure is greater than the pressure within the tan
52             % is incrementally increased and iterated in a while loop until mach number is equal to one
53
54             Inlet_entropy = entropy_inlet(i,j+1);
55             Inlet_stagnation_enthalpy = h_inlet(i,j+1);
56             P_guess = Pressure_exit;
57
58             if mach_exit(i,j+1) > 1
59                 Pressure_exit = find_exit_pressure(Inlet_stagnation_enthalpy,Inlet_entropy,Fluid{i},P_guess, ref
60                 sound_exit(i,j+1) = refpropm('A','P',Pressure_exit,'S',Inlet_entropy,Fluid{i}, refpropdir);
61                 h_static_exit(i,j+1) = refpropm('H','P',Pressure_exit,'S',Inlet_entropy,Fluid{i}, refpropdir);

```



```

62         visc_exit(i,j+1) = refpropm('V','P',Pressure_exit,'S',Inlet_entropy,Fluid{i}, refprop
63         mach_exit(i,j+1) = sqrt(2*(h_inlet(i,j+1)-h_static_exit(i,j+1))/sound_exit(i,j+1)^2)
64     end
65
66     %% Calculation of the mass flow rate into the tank(s)
67
68     rho_exit(i,j+1) = refpropm('D','P',Pressure_exit,'S',Inlet_entropy,Fluid{i}, refpropdir)
69     vel_exit(i,j+1) = mach_exit(i,j+1)*sound_exit(i,j+1);
70     Re_exit_isentropic(i,j+1) = rho_exit(i,j+1) *d_inlet*vel_exit(i,j+1)/visc_exit(i,j+1);
71     cd(i,j+1) = 1 + J/(Re_exit_isentropic(i,j+1)^(0.25));
72     mfr(i,j+1) = cd(i,j+1)*rho_exit(i,j+1)*vel_exit(i,j+1)*A_inlet;
73     Re_entrance_actual(i,j+1) = 4*mfr(i,j+1)/(pi*d_inlet*visc_exit(i,j+1));
74     dM_inlet = mfr(i,j+1)*dt;
75 end
76
77 %% Heat transfer calculations & caluculations of the thermodynamic properties of the gas in t
78 if l_d(i) <= 3 | blnOneZone{i} == 1
79
80     Nus(i,j+1) = a_1*Re_entrance_actual(i,j+1)^(b_1); % Nusselt number a
81     k_gas(i,j+1) = refpropm('L','T',Temp_gas(i,j),'P',P_gas(i,j),Fluid{i}, refpropdir); % T
82     heat_coef_forced(i,j+1) = Nus(i,j+1)*k_gas(i,j+1)/d_tank(i); % Calculation of t
83
84     if Inner_wall_boundary(i) == 1
85         Qsurf(i,j+1) = -dt*surf_area(i)*heat_coef_forced(i,j+1)*(Temp_gas(i,j)-Inner_temp_wa
86     else
87         Qsurf(i,j+1) = -dt*surf_area(i)*heat_coef_forced(i,j+1)*(Temp_gas(i,j)-Temp_wall{i}(
88         Temp_wall{i}(1,j+1) = Temp_wall{i}(1,j) + CFL_liner(i)*(Temp_wall{i}(2,j)- Temp_wall{
89
90         if Outer_wall_boundary(i)==1
91             Temp_wall{i}(number_of_gridpoints(i),j+1) = Outer_temp_wall_isothermal(i);
92         else
93             Temp_wall{i}(number_of_gridpoints(i),j+1) = Temp_wall{i}(number_of_gridpoints(i)
94         end
95         % Computation of the temperature of the struture of the tank(s)
96         for k=2:number_of_gridpoints(i)-1
97             if (k>=2)&&(k<=int_pt_liner_laminate(i)-1)
98                 Temp_wall{i}(k,j+1) = Temp_wall{i}(k,j)+CFL_liner(i)*(Temp_wall{i}(k+1,j)-2*
99             elseif (k>=int_pt_liner_laminate(i)+1)&&(k<=number_of_gridpoints(i)-1)
100                 Temp_wall{i}(k,j+1) = Temp_wall{i}(k,j)+CFL_laminate(i)*(Temp_wall{i}(k+1,j)
101             else
102                 Temp_wall{i}(k,j+1) = (cond_laminate(i)*(Temp_wall{i}(k+1,j)+CFL_laminate(i)
103             end
104         end
105     end
106     m_gas(i,j+1) = m_gas(i,j) + dM_inlet; % Mas
107     Ugas(i,j+1)=Ugas(i,j)+Qsurf(i,j+1)+h_inlet(i,j+1)*dM_inlet; % Int
108     u_gas(i,j+1)= Ugas(i,j+1)/m_gas(i,j+1); % Spe
109     rho_gas(i,j+1)=m_gas(i,j+1)/vol_tank(i); % Den
110     P_gas(i,j+1) = refpropm('P','D',rho_gas(i,j+1),'U',u_gas(i,j+1),Fluid{i}, refpropdir);
111     Temp_gas(i,j+1) = refpropm('T','D',rho_gas(i,j+1),'U',u_gas(i,j+1),Fluid{i}, refpropdir)
112
113 else
114     Re_compression(i,j+1) = Re_entrance_actual(i,j+1)*(d_inlet/d_tank(i)); % Rey
115
116     Nus_zone1{i}(j+1) = a_1*Re_entrance_actual(i,j+1)^(b_1); % Nus
117     Nus_zone2{i}(j+1) = c_1*Re_compression(i,j+1)^(d_1); % Nus
118
119     k_gas_zone1{i}(j+1) = refpropm('L','T',Temp_gas_zone1{i}(j),'P',P_gas_zone1{i}(j),Fluid
120     k_gas_zone2{i}(j+1) = refpropm('L','T',Temp_gas_zone2{i}(j),'P',P_gas_zone2{i}(j),Fluid
121
122     heat_coef_forced_zone1{i}(j+1) = Nus_zone1{i}(j+1)*k_gas_zone1{i}(j+1)/d_tank(i);
123     heat_coef_forced_zone2{i}(j+1) = Nus_zone2{i}(j+1)*k_gas_zone2{i}(j+1)/l_zone2_total(i)
124
125     % Step 1. Equating the respecting values of zone 1 and zone 2 to
126     % matrices with 'similar' names
127

```

```

128     Vgas(1)=volume_zone1(i);
129     Vgas(2)=volume_zone2(i);
130     Mgas(1)=m_gas_zone1{i}(j);
131     Mgas(2)=m_gas_zone2{i}(j);
132     Ugas_twozone(1)=u_gas_zone1{i}(j)*Mgas(1);
133     Ugas_twozone(2)=u_gas_zone2{i}(j)*Mgas(2);
134     Asurf(1)=surface_area_zone1(i);
135     Asurf(2)=surface_area_zone2(i);
136     Tgas(1)=Temp_gas_zone1{i}(j);
137     Tgas(2)=Temp_gas_zone2{i}(j);
138     if Inner_wall_boundary(i) == 1
139         Twall(1,1)=Inner_temp_wall_isothermal(i);
140         Twall(2,1)=Inner_temp_wall_isothermal(i);
141     else
142         Twall(1,1)=Temp_wall_zone1{i}(1,j);
143         Twall(2,1)=Temp_wall_zone2{i}(1,j);
144     end
145     % Step 2: apply the change of internal energy due to heat transfer and mass
146     % input through nozzle:
147
148     dM_inlet = mfr(i,j+1)*dt;
149
150     Qsurf(1)=- dt*Asurf(1)*(heat_coef_forced_zone1{i}(j+1))*(Tgas(1)-Twall(1,1));
151     Qsurf(2)=- dt*Asurf(2)*(heat_coef_forced_zone2{i}(j+1))*(Tgas(2)-Twall(2,1));
152
153     Ugas_twozone(1)=Ugas_twozone(1)+Qsurf(1)+h_inlet(i,j+1)*dM_inlet;
154     Ugas_twozone(2)=Ugas_twozone(2)+Qsurf(2);
155
156     Mgas(1)=Mgas(1)+dM_inlet;
157     Mgas(2)=Mgas(2);
158
159     for m=1:2
160         hgas(m)=refpropm('H','D',Mgas(m)/Vgas(m),'U',Ugas_twozone(m)/Mgas(m),Fluid{i}, refpropdir);
161     end
162
163
164     % Step 2: Find the amount of mass that needs to be transferred from zone 1
165     % to zone 2 to equalise their pressure
166     % (we assume forward Euler integration, therefore we use the specific
167     % enthalpies h from the start of the timestep. We provide enthalpies for
168     % both zones in case the flow gets reversed).
169
170     dM_guess = dM_inlet*(volume_zone2(i)/(volume_zone1(i)+volume_zone2(i))) ;
171     dM_12 = find_dM_12(hgas,Vgas,Mgas,Ugas_twozone,Fluid{i},dM_guess, refpropdir);
172
173     % Step 3: Apply this change to the mass and update all properties:
174
175     m_gas_zone1{i}(j+1)=Mgas(1)-dM_12;
176     m_gas_zone2{i}(j+1)=Mgas(2)+dM_12;
177
178     u_gas_zone1{i}(j+1)=(Ugas_twozone(1)-max(0,dM_12)*hgas(1)-min(0,dM_12)*hgas(2))/m_gas_zone1{i}(j+1);
179     u_gas_zone2{i}(j+1)=(Ugas_twozone(2)+max(0,dM_12)*hgas(1)+min(0,dM_12)*hgas(2))/m_gas_zone2{i}(j+1);
180
181     rho_gas_zone1{i}(j+1)=m_gas_zone1{i}(j+1)/volume_zone1(i);
182     rho_gas_zone2{i}(j+1)=m_gas_zone2{i}(j+1)/volume_zone2(i);
183
184     Temp_gas_zone1{i}(j+1)=refpropm('T','D',rho_gas_zone1{i}(j+1),'U', u_gas_zone1{i}(j+1),Fluid{i}, refpropdir);
185     Temp_gas_zone2{i}(j+1)=refpropm('T','D',rho_gas_zone2{i}(j+1),'U', u_gas_zone2{i}(j+1),Fluid{i}, refpropdir);
186
187     P_gas_zone1{i}(j+1)=refpropm('P','D',rho_gas_zone1{i}(j+1),'U', u_gas_zone1{i}(j+1),Fluid{i}, refpropdir);
188     P_gas_zone2{i}(j+1)=refpropm('P','D',rho_gas_zone2{i}(j+1),'U', u_gas_zone2{i}(j+1),Fluid{i}, refpropdir);
189
190     m_gas(i,j+1) = m_gas_zone1{i}(j+1) + m_gas_zone2{i}(j+1);
191     rho_gas(i,j+1) = m_gas(i,j+1)/vol_tank(i);
192     u_gas(i,j+1)= (u_gas_zone1{i}(j+1)*m_gas_zone1{i}(j+1)+ u_gas_zone2{i}(j+1)*m_gas_zone2{i}(j+1))/m_gas(i,j+1);
193     Ugas(i,j+1) = u_gas(i,j+1)*m_gas(i,j+1);

```

```

194     Temp_gas(i,j+1) = refpropm('T','D',rho_gas(i,j+1),'U',u_gas(i,j+1),Fluid{i}, refpropdir
195     P_gas(i,j+1) = refpropm('P','D',rho_gas(i,j+1),'U',u_gas(i,j+1),Fluid{i}, refpropdir);
196
197     if Inner_wall_boundary(i) == 1
198         Qsurf_zone1{i}(j+1) = -dt*surface_area_zone1(i)* heat_coef_forced_zone1{i}(j+1)*(Tem
199         Qsurf_zone2{i}(j+1) = -dt*surface_area_zone2(i)* heat_coef_forced_zone2{i}(j+1)*(Tem
200     else
201         Qsurf_zone1{i}(j+1) = -dt*surface_area_zone1(i)* heat_coef_forced_zone1{i}(j+1)*(Tem
202         Qsurf_zone2{i}(j+1) = -dt*surface_area_zone2(i)* heat_coef_forced_zone2{i}(j+1)*(Tem
203
204         Temp_wall_zone1{i}(1,j+1) = Temp_wall_zone1{i}(1,j)+ CFL_liner(i)*(Temp_wall_zone1{i}
205         Temp_wall_zone2{i}(1,j+1) = Temp_wall_zone2{i}(1,j)+ CFL_liner(i)*(Temp_wall_zone2{i}
206
207     if Outer_wall_boundary(i)==1
208         Temp_wall_zone1{i}(number_of_gridpoints(i),j+1) = Outer_temp_wall_isothermal(i);
209         Temp_wall_zone2{i}(number_of_gridpoints(i),j+1) = Outer_temp_wall_isothermal(i);
210     else
211         Temp_wall_zone1{i}(number_of_gridpoints(i),j+1) = Temp_wall_zone1{i}(number_of_g
212         Temp_wall_zone2{i}(number_of_gridpoints(i),j+1) = Temp_wall_zone2{i}(number_of_g
213     end
214     % Computation of the temperature of the struture of the tank(s)
215     for k=2:number_of_gridpoints(i)-1
216         if (k>=2)&&(k<=int_pt_liner_laminate(i)-1)
217             Temp_wall_zone1{i}(k,j+1) = Temp_wall_zone1{i}(k,j)+CFL_liner(i)*(Temp_wall_
218             Temp_wall_zone2{i}(k,j+1) = Temp_wall_zone2{i}(k,j)+CFL_liner(i)*(Temp_wall_
219         elseif (k>=int_pt_liner_laminate(i)+1)&&(k<=number_of_gridpoints(i)-1)
220             Temp_wall_zone1{i}(k,j+1) = Temp_wall_zone1{i}(k,j)+CFL_laminate(i)*(Temp_wa
221             Temp_wall_zone2{i}(k,j+1) = Temp_wall_zone2{i}(k,j)+CFL_laminate(i)*(Temp_wa
222         else
223             Temp_wall_zone1{i}(k,j+1) = (cond_laminate(i)*(Temp_wall_zone1{i}(k+1,j)+CFL
224             Temp_wall_zone2{i}(k,j+1) = (cond_laminate(i)*(Temp_wall_zone2{i}(k+1,j)+CFL
225         end
226     end
227 end
228
229     end
230
231     end
232 end

```

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