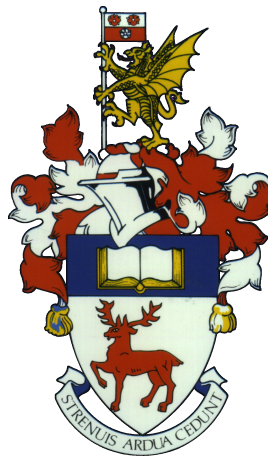


1 **Novel Approaches to Fast Filling of Hydrogen Cylinders**

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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;

13

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

15

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

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

25

Abstract

26

This is the abstract.

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61 **References**

11

62 **Acronyms**

63 **CFD** Computational Fluid Dynamics

64 **Todo list**

65	Reword	1
66	Update with actual options considered at end of project	1
67	Cite	2
68	Fill	2
69	cite: http://www.epotek.com/site/files/Techtips/pdfs/tip23.pdf	2
70	Citation	3
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72	fill	4
73	Fill Section once work on optimization starts.	4
74	Citation	6
75	define short and long cylinders at some point	6
76	Play around with this perhaps?	6
77	General stuff:	
78	- Check tense and person	
79	- Check for repetition	
80	- Check for excessive verbosity	6

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. 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 that 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 the faster refueling of hydrogen cylinders. To this end, this project will build upon a model of filling a hydrogen cylinder which has already been developed by members of the department in order 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 analyzing the temperature of the structure, and see 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 Vehicles and objectives

We must firstly consider what real-world relevance of this project is. As explained in Section 1, the hydrogen cylinders being considered are for road vehicles. Although still an emerging technology, the basic functioning of a hydrogen fueled cylinders is relatively well established. They store compressed hydrogen in fuel tanks at high pressures, 35 and 70 MPa are the two current standards for pressure. This hydrogen is then used in the fuel cell and converted into electricity,, which can be used directly by the electric motor or stored on onboard batteries. It therefore follows that the objectives of the hydrogen storage system are several:

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

These have certain implications. Firstly, 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, which inevitably leads to higher temperatures. These higher temperatures are problematic due to material constraints as explained below in Section 2.1.1. Indeed, they lead to longer filling times as heat is allowed to dissipate through the tank walls. This leads to the desire to optimize filling patterns and develop other solutions to minimize temperature rise when filling to high pressures.

2.1.1 Material constraints

The main reason that a problem exists, and consequently this paper (and much other work) is being undertaken, is the material limitations that exist in hydrogen cylinders. Indeed, the cylinders that are used for high pressure scenarios such as the one we are presented with, are constructed with a composite material such as carbon fibre or glass/aramid fibre. In addition, they have a liner that is made out of metal, typically aluminum, in Type III cylinders, and out of a thermoplastic material for Type IV cylinders. 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.

2.2 Previous work

We must first establish a baseline of previous work that has been conducted in this field, and subsequently analyze the shortcomings that exist in order to direct the research.

149 2.2.1 Modeling Work

150 A large amount of research has been conducted using multidimensional analysis, especially using
151 Computational Fluid Dynamics (CFD). Indeed, there is myriad papers describing different methods
152 and setups, such as Dicken and Mérida's work, which uses the standard k- ϵ turbulence model and the
153 Redlich-Kwong real gas equation of state for real gas properties [1]. Some of these models use more
154 advanced property models, such as the model presented by Zhao et al., which employs REFPROP
155 (see Section 2.5.3) in order to have more precise real gas properties [2].

156 2.2.2 Experimental work

157 Several papers describe experimental work that has been conducted regarding the fast-filling of
158 hydrogen cylinders, in particular comparing the results to simulations. Dicken and Mérida's work
159 indicates that the temperature inside the cylinder is rather uniform [3]. This claim is not, however
160 supported by the work of Zheng et al nor that of Woodfield et al [4], wherein large discrepancies
161 among gas temperatures in different regions of the cylinder are found.

162 2.2.3 Analysis

163 The simulation work that has been conducted can be, in broad terms, divided into complex CFD
164 models and more simplified 0-dimensional models. It is important analyze the difference between
165 these two systems. The main advantage of reduced dimension models is that they are much less
166 computationally expensive. This, in turn, means it can be incorporated as part of a larger analysis,
167 in which it must be run multiple times, such as optimization routines or probabilistic whole station
168 models.

169 Reduced dimension models assume a constant gas temperature, which, as outlined in Section
170 2.2.2, is supported by some experimental work, but refuted by others. For this reason, more research
171 should be conducted to validate the uniform gas temperature approximation.

172 2.3 Cylinder filling models

173 Several ways of modelling the cylinder can be considered when analysing their filling, with varying
174 complexity and accuracy.

175 2.3.1 Zonal

176 A zonal model, also referred to as a 0-dimensional model, refers to models that consider the gas
177 inside the cylinder as the control volume, with homogenous properties. This allows for simpler
178 calculations and much lower computational time.

179 2.3.2 Multidimensional

180 More complex multidimensional models can be created, either 2D axisymmetric models or full 3D
181 models. 2D models will not include the effects of gravity or buoyancy, but these can be considered

negligible, and the computational expense of full 3D simulations is rarely justifiable as the gains in accuracy are very small.

fill

2.4 Heat transfer models

In order to successfully analyse the behaviour of the system as a whole we must consider several local heat transfer methods that occur at different places inside of the cylinder.

2.4.1 Impinging jet

The first behaviour that we will consider is that of an impinging jet of fluid onto a surface.

FIGURE 1: Impinging jet

{fig:impinging_jet}

2.4.2 Pipe flow

A second behaviour that we will consider is that of pipe flow. This behaviour has been the focus of much research, as it is arguably the most common mode of heat transfer that occurs in fluid systems.

2.4.3 Turbulent Jets

Lastly, we must also consider turbulent jets, as there will be such a situation at the exit of the nozzle. [5]

2.5 Methodology

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

2.5.1 Optimization

Fill Section
once work on
optimization
starts.

2.5.2 Non-dimensioning

One of the fundamental principals 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.

205 2.5.3 Numerical methods

206 **Integrating ODEs** An central part of solving unsteady heat transfer problems involves integrating
 207 ODEs, as will be seen in Section 3. One of the simplest methods available, both conceptually and
 208 in terms of ease of implementing in code, is forward Euler time integration. It can be informally
 209 described as follows: given a function that can be defined by:

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

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

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

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

218 The property model that will be employed throughout this analysis is REFPROP, a tool developed
 219 by the National Institute of Standards and Technology [6]. It uses values of critical and triple points
 220 together with equations for the thermodynamic and transport properties to calculate the state points
 221 of fluids.

222 3 Formulation

223 3.1 Heat transfer across cylinder

224 The main mode of heat transfer that occurs in the cylinder and that will be used throughout this report
 225 is heat conduction through the wall of the cylinder. This is modeled using:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad (3.1)$$

226 where a is the thermal diffusivity, which is defined by :

$$\alpha = \frac{k}{\rho c} \quad (3.2)$$

227 where k is the material's thermal conductivity, ρ is the density of the material, and c is the specific
 228 heat capacity of the material. This differential equation will be solved using forward Euler time
 229 integration as described in Section 2.5.3.

3.2 Gas 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:

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

where ρ_{exit} , d_{inlet} , u_{exit} , and μ_{exit} are determined using real gas models as described in Section 2.5.3. In order to find the real mass flow an empirical discharge coefficient is employed:

$$\text{CD} = \frac{\dot{m}_{\text{in}}}{\dot{m}_{\text{ideal}}} = A + B \text{Re}_{\text{ideal}} \quad (3.4)$$

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 [1], and uses the following values:

$$A = 0.938, \quad B = -2.71 \quad (3.5)$$

3.3 Hysteresis

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 of course is a time delay, measured to be approximately 2 seconds for short cylinders. This assumption is acceptable for stable inflows, 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:

$$\frac{d}{dt}(\text{Nu}) = \frac{\text{Nu}_{ss} - \text{Nu}}{\tau} \quad (3.6)$$

3.4 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 2.1.1. A simple method of throttling, with the flow stopping at the designated maximum temperature, 85 °C, and the flow restarting at a chosen temperature, in this case 75 °C.

3.5 Optimization

Citation

define short and long cylinders at some point

Play around with this perhaps?

General stuff:
- Check tense and person
- Check for repetition
- Check for excessive verbosity

254 **Appendices**255 **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 a
12 % and calculating the stagnation enthalpy and entropy
13
14 for j = 1:maxt
15     time(j+1) = (j)*dt; % Time as filling process
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
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}, refproppdir)
35         entropy_inlet(i,j+1) = refpropm('S','T',Temp_inlet(i,j+1),'P',P_inlet(i,j+1),Fluid{i}, refproppdir)
36
37         %% Determine which pressure to use at the exit of the delivery pipe which is dependent upon
38
39         if l_d(i) > 3 && blnOneZone{i} == 0 % The length-to-diameter ratio of the tank(s) d
40             Pressure_exit = P_gas_zone1{i}(j); % The pressure at the exit of the delivery pipe is
41         else
42             Pressure_exit = P_gas(i,j); % The pressure at the exit of the delivery pipe is
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}, refproppdir)
47             h_static_exit(i,j+1) = refpropm('H','P',Pressure_exit,'S',entropy_inlet(i,j+1),Fluid{i}, refproppdir)
48             visc_exit(i,j+1) = refpropm('V','P',Pressure_exit,'S',entropy_inlet(i,j+1),Fluid{i}, refproppdir)
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);
50
51             %% If Mach number is greater than one, the exit pressure is greater than the pressure wi
52             % is incrementally increased and iterated in a while loop until mach number is equal to
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},
60                 sound_exit(i,j+1) = refpropm('A','P',Pressure_exit,'S',Inlet_entropy,Fluid{i}, refproppdir)
61                 h_static_exit(i,j+1) = refpropm('H','P',Pressure_exit,'S',Inlet_entropy,Fluid{i}, refproppdir)

```

```

62         visc_exit(i,j+1) = refpropm('V','P',Pressure_exit,'S',Inlet_entropy,Fluid{i}, refpropdir);
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); % Co
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); % Calcul
70     Re_exit_isentropic(i,j+1) = rho_exit(i,j+1) *d_inlet*vel_exit(i,j+1)/visc_exit(i,j+1); % Calcul
71     cd(i,j+1) = I + J/(Re_exit_isentropic(i,j+1)^(0.25)); % Calcul
72     mfr(i,j+1) = cd(i,j+1)*rho_exit(i,j+1)*vel_exit(i,j+1)*A_inlet; % Calcul
73     Re_entrance_actual(i,j+1) = 4*mfr(i,j+1)/(pi*d_inlet*visc_exit(i,j+1)); % Calcul
74     dM_inlet = mfr(i,j+1)*dt; % Amount
75 end
76
77 %% Heat transfer calculations & caluculations of the thermodynamic properties of the gas in the tank(s) v
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 and Reynolds
81     k_gas(i,j+1) = refpropm('L','T',Temp_gas(i,j),'P',P_gas(i,j),Fluid{i}, refpropdir); % Thermal condu
82     heat_coef_forced(i,j+1) = Nus(i,j+1)*k_gas(i,j+1)/d_tank(i); % Calculation of the heat tran
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_wall_isotherma
86     else
87         Qsurf(i,j+1) = -dt*surf_area(i)*heat_coef_forced(i,j+1)*(Temp_gas(i,j)-Temp_wall{i}(1,j));
88         Temp_wall{i}(1,j+1) = Temp_wall{i}(1,j) + CFL_liner(i)*(Temp_wall{i}(2,j)- Temp_wall{i}(1,j) - Qs
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),j)+2*CFL_l
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*Temp_wall{i}
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)-2*Temp_wall
101         else
102             Temp_wall{i}(k,j+1) = (cond_laminate(i)*(Temp_wall{i}(k+1,j)+CFL_laminate(i)*(Temp_wall
103         end
104     end
105 end
106 m_gas(i,j+1) = m_gas(i,j) + dM_inlet; % Mass of gas in
107 Ugas(i,j+1)=Ugas(i,j)+Qsurf(i,j+1)+h_inlet(i,j+1)*dM_inlet; % Internal energy
108 u_gas(i,j+1)= Ugas(i,j+1)/m_gas(i,j+1); % Specific energy
109 rho_gas(i,j+1)=m_gas(i,j+1)/vol_tank(i); % Density of the
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)); % Reynolds number
115
116     Nus_zone1{i}(j+1) = a_1*Re_entrance_actual(i,j+1)^(b_1); % Nusselt number
117     Nus_zone2{i}(j+1) = c_1*Re_compression(i,j+1)^(d_1); % Nusselt number
118
119     k_gas_zone1{i}(j+1) = refpropm('L','T',Temp_gas_zone1{i}(j),'P',P_gas_zone1{i}(j),Fluid{i}, refprop
120     k_gas_zone2{i}(j+1) = refpropm('L','T',Temp_gas_zone2{i}(j),'P',P_gas_zone2{i}(j),Fluid{i}, refprop
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)*(Temp_gas_zone1{i}(j+1)-Temp_gas_zone2{i}(j+1));
199     Qsurf_zone2{i}(j+1) = -dt*surface_area_zone2(i)* heat_coef_forced_zone2{i}(j+1)*(Temp_gas_zone2{i}(j+1)-Temp_gas_zone1{i}(j+1));
200 else
201     Qsurf_zone1{i}(j+1) = -dt*surface_area_zone1(i)* heat_coef_forced_zone1{i}(j+1)*(Temp_gas_zone1{i}(j+1)-Temp_gas_zone2{i}(j+1));
202     Qsurf_zone2{i}(j+1) = -dt*surface_area_zone2(i)* heat_coef_forced_zone2{i}(j+1)*(Temp_gas_zone2{i}(j+1)-Temp_gas_zone1{i}(j+1));
203
204     Temp_wall_zone1{i}(1,j+1) = Temp_wall_zone1{i}(1,j)+ CFL_liner(i)*(Temp_wall_zone1{i}(2,j)-Temp_wall_zone1{i}(1,j));
205     Temp_wall_zone2{i}(1,j+1) = Temp_wall_zone2{i}(1,j)+ CFL_liner(i)*(Temp_wall_zone2{i}(2,j)-Temp_wall_zone2{i}(1,j));
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_gridpoints(i),j);
212     Temp_wall_zone2{i}(number_of_gridpoints(i),j+1) = Temp_wall_zone2{i}(number_of_gridpoints(i),j);
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_zone1{i}(k+1,j)-Temp_wall_zone1{i}(k,j));
218         Temp_wall_zone2{i}(k,j+1) = Temp_wall_zone2{i}(k,j)+CFL_liner(i)*(Temp_wall_zone2{i}(k+1,j)-Temp_wall_zone2{i}(k,j));
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_wall_zone1{i}(k+1,j)-Temp_wall_zone1{i}(k,j));
221         Temp_wall_zone2{i}(k,j+1) = Temp_wall_zone2{i}(k,j)+CFL_laminate(i)*(Temp_wall_zone2{i}(k+1,j)-Temp_wall_zone2{i}(k,j));
222     else
223         Temp_wall_zone1{i}(k,j+1) = (cond_laminate(i)*(Temp_wall_zone1{i}(k+1,j)+CFL_laminate(i)*(Temp_wall_zone1{i}(k+2,j)-Temp_wall_zone1{i}(k+1,j)));
224         Temp_wall_zone2{i}(k,j+1) = (cond_laminate(i)*(Temp_wall_zone2{i}(k+1,j)+CFL_laminate(i)*(Temp_wall_zone2{i}(k+2,j)-Temp_wall_zone2{i}(k+1,j)));
225     end
226 end
227 end
228
229 end
230
231 end
232 end

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