Optimization of the refueling for hydrogen gas tanks
IMI departement project

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Motivation: reducing costs and real time computations

Hydrogen vehicles represent a crucial part of the strategy to reduce greenhouse gas emissions linked to transport. However, to contribute to such a strategy the technology needs to be optimal for the users. In order for the user to not be bothered by this type of vehicle, the refueling time of the tank must be in the same range as for a thermic vehicle. However, a problem arises: **during hydrogen refueling, the high pressure (700 bara) in the dispensers -caused by the speed at which we wish to refuel- induces a significant rise of the tank's temperature**. The tank's walls being made of composite materials which cannot withstand temperatures above 85°C. This leads to the two following situations: either the refill must be slower and heat loss allows the temperature to remain below the 85°C threshold or **the gas must be pre-cooled before entering the tank while keeping a low refueling time**.

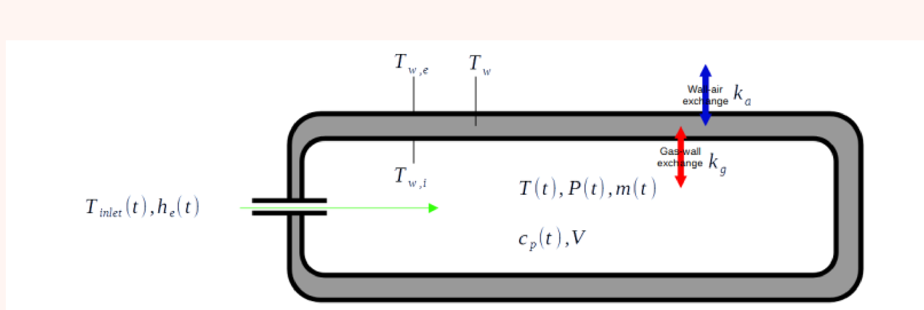
However, pre-cooling is costly and its use must be determined for each particular case as the tank is not at the same temperature in every car and at every time. For the sake of this project, we decided to fix a constant refueling time of 5 minutes, which is the average time spent at a gas station. Under these settings, the project consists in **optimizing the electrical consumed for the pre-cooling process under the constraint of having the temperature inside the tank below 85°C at each time**.

Key steps

- **Thermal modeling of gas filling:** Understanding the physical laws used to model the tank and the Hydrogen refueling.
- **Combination of both simulation and optimization solvers:** Evaluating the best choices based on performances, robustness, adaptability...
- **Producing a real time computing solution:** Given some input parameters (duration, pressure expected, constraints...), an optimised injection temperature profile must be computed in real time.

The 0D/1D model used for the modeling

The **0D/1D models**, commonly used in various industries including gas production and distribution like at Air Liquide are used to simulate and understand physical systems where spatial dimensions can be simplified while allowing a certain computational simplicity. A 0D/1D model treats the system (the interior of the tank) as a singular point where processes unfold instantaneously and uniformly in which we introduce variation along a single spatial dimension (1D in tank walls).



Equations of the problem

Boundary and initial conditions

Temperatures of the tank walls are the same of the ambient temperature for the outer surface and gaz temperature for the interior surface.

Initial injection temperture is fixed at the ambient temperature

Pressure

Constant rise in pressure inside the tank

$$P(t) = P_0 + P_{var} \cdot t \tag{1}$$

Gas temperature

The hydrogen enters the tank at the pre-cooled temperature profile $T_{inlet}(t)$. $h(t) = H(T(t), P(t))$ is the gas enthalpy and $h_e(t) = H(T_{inlet}(t), P(t))$ the inlet enthalpy and we have this differential equation to describe the gas in the tank:

$$m \cdot c_p \cdot \frac{dT}{dt} = V \cdot \beta \cdot T \cdot \frac{dP}{dt} + k_g \cdot S_i \cdot (T_{w,i} - T) + \frac{dm}{dt} \cdot (h_e - h) \tag{2}$$

Diffusion in the tank walls

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \tag{3}$$

Where α is the thermal diffusivity of the material, T is the temperature, t is time, and x is the spatial dimension normal to the tank walls

Mass

$Z(T, P)$ is the compressibility factor of the gas

$$P \cdot V \cdot M = m \cdot R \cdot Z(T, P) \cdot T \tag{4}$$

Energy cost

$$E = \int_0^{t_f} (h_{in} - h_{amb}) \cdot \frac{dm}{dt} dt \tag{5}$$

Optimization problem

The project lies in finding "the" best injection temperature profile, in the sense of the profile with the lowest energy costs.

Problem while searching for a discretized injection temperature profile

$$\begin{aligned} \min_{T_{inlet}:[0,t_0] \to [T_{inlet}^{min}, T_{inlet}^{max}]} \quad & E = \int_0^{t_f} (h_{in} - h_{amb}) \cdot \frac{dm}{dt} dt \\ \text{s.t.} \quad & \sup_{t \in [0,t_0]} T(t) \leq T_{max} \\ & \sup_{t \in [0,t_0]} \left| \frac{dT_{inlet}}{dt} \right| \leq 2K \cdot s^{-1} \\ & T(0) = T_{amb} \\ \text{where} \quad & h_(in), m, T \text{ are solutions of } (1):(5) \end{aligned}$$

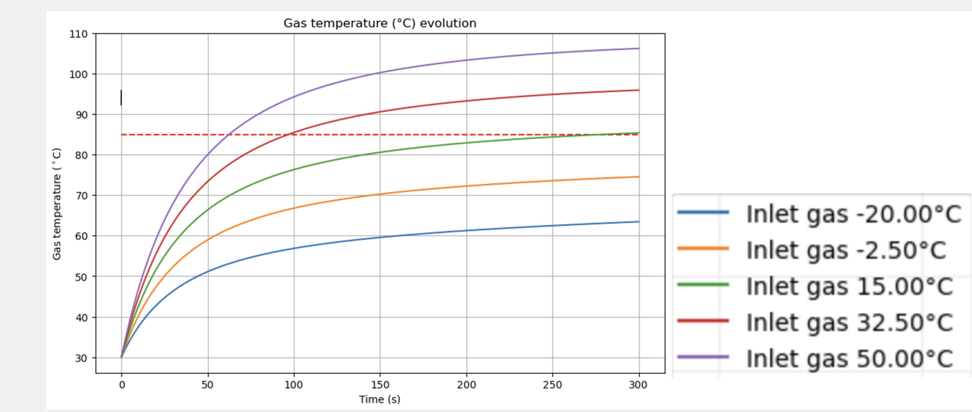
The difficulty of the above optimisation problem lies in the fact that it is not expressed in standard form. The constraints relate to the solution of a system of differential equations.

In order to simplify the optimization problem, we first optimize on a finite number N of points and then interpolate.

Optimization on a set of predifined parametric functions

Another method envisaged to reduce the number of parameters is to optimize on a set of predifined parametric functions for the entry temperature.

Solving the system of differential equations for constant temperature filling

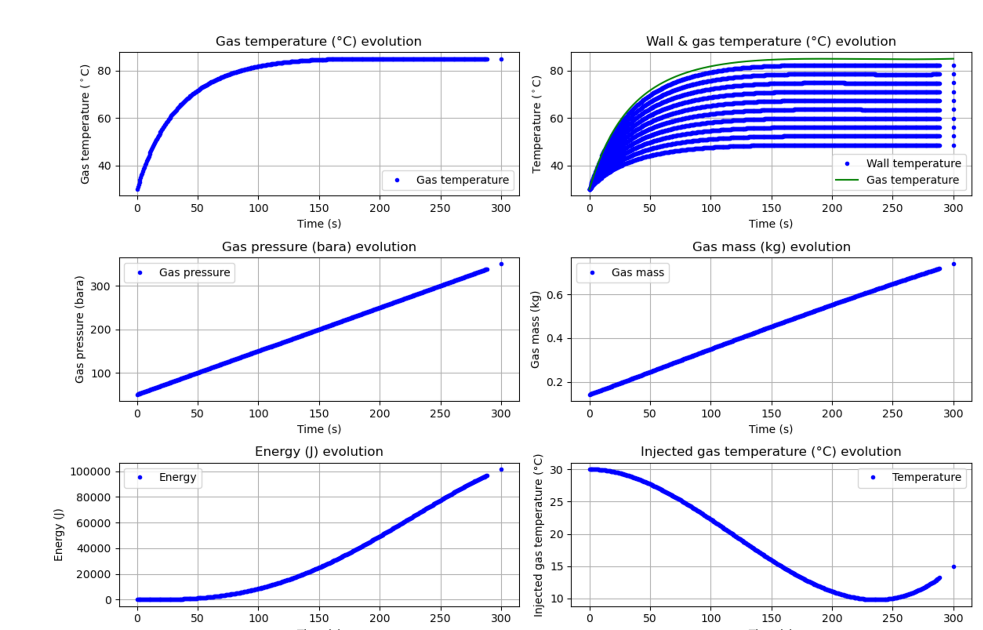


Orders of magnitude

- Refueled tank pressure : 350-700 bara
- Maximal gas temperature : 85°C
- Refueling time : 300 s
- Cooling speed : -2 $K.s^{-1}$
- Non optimized profiles energy cost : 300 kJ
- Optimized profiles energy cost : 100 kJ

Optimization's first results

Optimization with 10 interpolation points (where the first is fixed at room temperature) gives us the profile at bottom right, leading to an energy value of $101kJ$.



Next stages of the project and objectives

- Optimization on parametrical profiles for the entry temperature rather than interpolation (more robust ?).
- Improve the tracking of the convergence during the optimization process to improve the computational speed.
- Introduce more constraints such as the hydrogen injection speed, and testing on different initial condition (changing the pressure ramp, final pressure, refueling time...)

References

[1] From scipy.org. https://docs.scipy.org/doc/scipy/reference/optimize.minimize-neldermead.htmloptimize-minimize-neldermead.

[2] D. Baraldi P. Moretto T. Bourgeois, F. Ammouri. The temperature evolution in compressed gas filling processes: A review. *International Journal of Hydrogen Energy*, 43(4):2268–2292, 2018.