

Hydrogen has the potential to become a clean energy carrier when produced via electrolysis (green hydrogen). However, hydrogen storing is challenging due to the extremely low density. At room temperature and standard pressure, 1 kg of hydrogen gas occupies 12 m<sup>3</sup>. Therefore, H<sub>2</sub> must be compressed to make it practical for transport, fueling stations, and industrial use.

In this exercise we will study the compression cost of hydrogen and compare different techniques for hydrogen storage to see how this cost can be reduced.

## Part 1

In a single-stage compressor, two different methods can be used: adiabatic and isothermal compression.

In the isothermal compression, heat is removed to keep the temperature constant, hence, the compression work required is reduced. While in the adiabatic compression, no heat is removed, hence, the temperature increases, which requires more compression work. Isothermal compression is a slow process and is used for energy storage, while adiabatic compression is a fast process and is used in internal combustion engines as well as air conditioning and refrigeration.

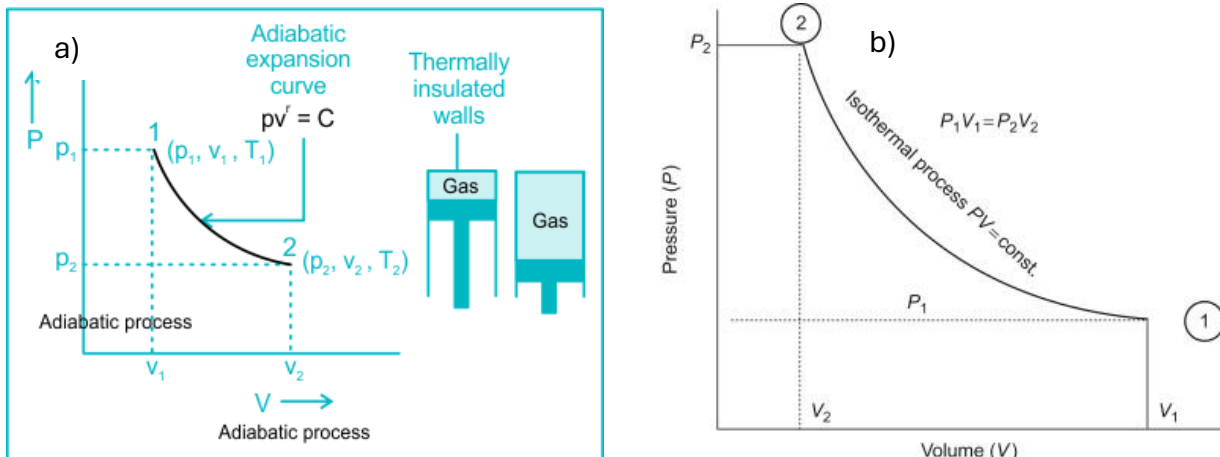


Figure 1: a) Adiabatic compression process b) Isothermal compression process

Knowing that the total work done on the gas is the integral of the pressure-volume work from  $V_1$  to  $V_2$  given as:

$$W = - \int_{V_1}^{V_2} P dV$$

- a) Using the ideal gas law, derive the adiabatic and isothermal compression work formula as a function of  $P_1$ ,  $P_2$ ,  $C_p$ ,  $T$ ,  $\gamma$  and  $\eta_c$ , where  $P_1$  and  $P_2$  are the initial and final pressures respectively,  $C_p$  the compressed gas specific heat,  $T$  the temperature,  $\gamma$  the specific heat ratio and  $\eta_c$  the compressor mechanical efficiency.
- b) Using the derived formulas, plot the adiabatic and isothermal compression cost curve as a function of pressure for  $H_2$ ,  $CH_4$ , and  $CO_2$ , when compressed from 1 bar up to 100 bar. Assume 70% mechanical efficiency.
- c) What observations can you make from the plots?

$$H_2: \begin{cases} c_{p,H_2} = 14'304 \left[ \frac{J}{kg \cdot K} \right] \\ \gamma_{H_2} = 1.41 \end{cases}$$

$$CH_4: \begin{cases} c_{p,H_2} = 2'191 \left[ \frac{J}{kg \cdot K} \right] \\ \gamma_{H_2} = 1.31 \end{cases}$$

$$CO_2: \begin{cases} c_{p,H_2} = 839 \left[ \frac{J}{kg \cdot K} \right] \\ \gamma_{H_2} = 1.30 \end{cases}$$

The total work done *on* the gas is the integral of the pressure-volume work from  $V_1$  to  $V_2$

$$W = - \int_{V_1}^{V_2} P dV$$

Using the adiabatic relationship, we know that  $P = \frac{C}{V^\gamma}$  where  $C = P_1 V_1^\gamma$

$$W = - \int_{V_1}^{V_2} \frac{P_1 V_1^\gamma}{V^\gamma} dV$$

Integrating  $V^{-\gamma}$  yields:

$$W = -P_1 V_1^\gamma \left[ \frac{V^{1-\gamma}}{1-\gamma} \right]_{V_1}^{V_2}$$

$$W = \frac{P_1 V_1^\gamma}{\gamma - 1} (V_2^{1-\gamma} - V_1^{1-\gamma})$$

Distribute  $P_1 V_1^\gamma$  (recognizing that  $P_1 V_1^\gamma = P_2 V_2^\gamma$ ):

$$W = \frac{P_2 V_2 - P_1 V_1}{\gamma - 1}$$

### Adapting to Temperature and Pressure

Apply the ideal gas law  $PV = nRT$  to substitute for  $PV$

$$W = \frac{nRT_2 - nRT_1}{\gamma - 1} = \frac{nR(T_2 - T_1)}{\gamma - 1}$$

To express this purely as a function of temperature and pressures, we use the temperature-pressure relation for adiabatic processes:

$$\frac{T_2}{T_1} = \left(\frac{P_2}{P_1}\right)^{\frac{\gamma-1}{\gamma}}$$

Isolating  $T_2$ :

$$T_2 = T_1 \left(\frac{P_2}{P_1}\right)^{\frac{\gamma-1}{\gamma}}$$

Substitute this back into the work equation:

$$W = \frac{nRT_1}{\gamma - 1} \left[ \left(\frac{P_2}{P_1}\right)^{\frac{\gamma-1}{\gamma}} - 1 \right]$$

Since  $R = C_p - C_v$ , and  $\gamma = \frac{C_p}{C_v}$ , we can substitute  $\frac{R}{\gamma-1} = \frac{C_p}{\gamma}$

Then, we get:

$$W = \frac{nC_p T_1}{\gamma} \left[ \left(\frac{P_2}{P_1}\right)^{\frac{\gamma-1}{\gamma}} - 1 \right] [J/kg]$$

Accounting for the mechanical efficiency of the compression process and converting to kWh, we get:

$$W = \frac{nC_p T_1}{3.6 \cdot 10^6 \gamma \eta_c} \left[ \left( \frac{P_2}{P_1} \right)^{\frac{\gamma-1}{\gamma}} - 1 \right] [kWh/kg]$$

Isothermal work:

Taking the same initial integral work formula and using ideal gas law to substitute the pressure, we get:

$$W = - \int_{V_1}^{V_2} \left( \frac{mRT}{V} \right) dV$$

$$W = - mRT \int_{V_1}^{V_2} \frac{1}{V} dV$$

$$W = - mRT [\ln(V)]_{V_1}^{V_2}$$

$$W = - mRT \ln \left( \frac{V_2}{V_1} \right)$$

By Boyle's Law, for a constant temperature process,  $P_1 V_1 = P_2 V_2$

Rearranging this gives the volume ratio in terms of the pressure ratio:

$$\frac{V_2}{V_1} = \frac{P_1}{P_2}$$

Substitute this ratio into the work equation:

$$W = - mRT \ln \left( \frac{P_1}{P_2} \right)$$

$$W = mRT \ln \left( \frac{P_2}{P_1} \right)$$

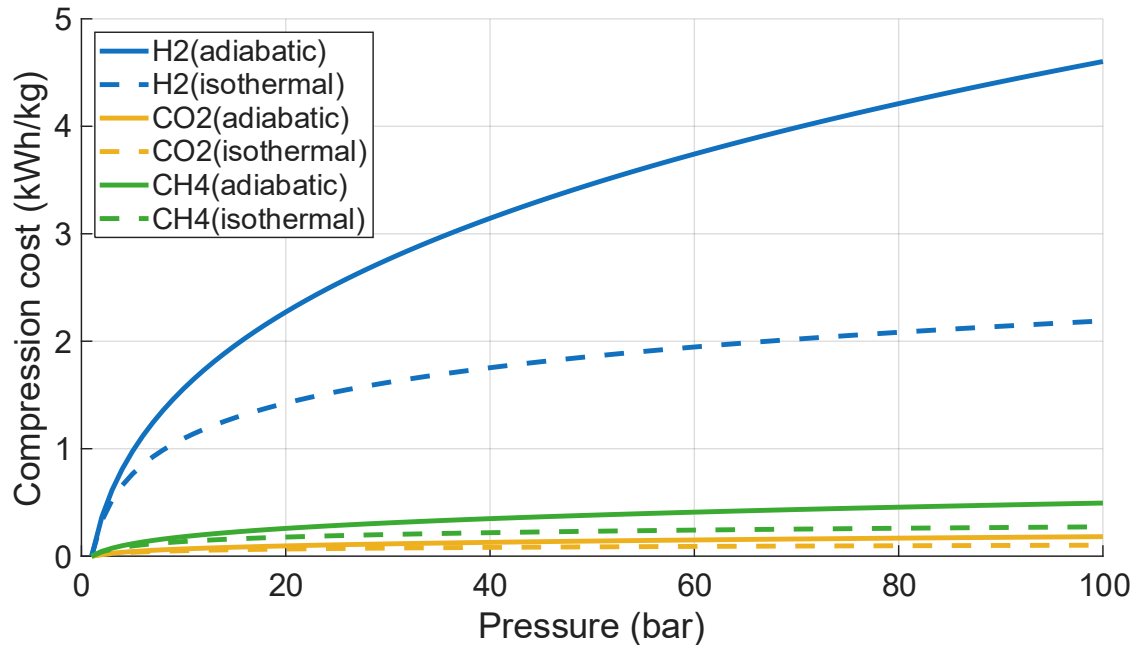
$$W_{comp, isot} = RT \ln \left( \frac{P_2}{P_1} \right) \left[ \frac{J}{kg} \right]$$

Considering the mechanical efficiency of the compressor and converting to kWh/kg, we get

$$W_{comp, isot} = \frac{RT}{(3.6 \cdot 10^6) \eta_c} \ln \left( \frac{P_2}{P_1} \right) \left[ \frac{kWh}{kg} \right]$$

The same equation can also be written as follows:

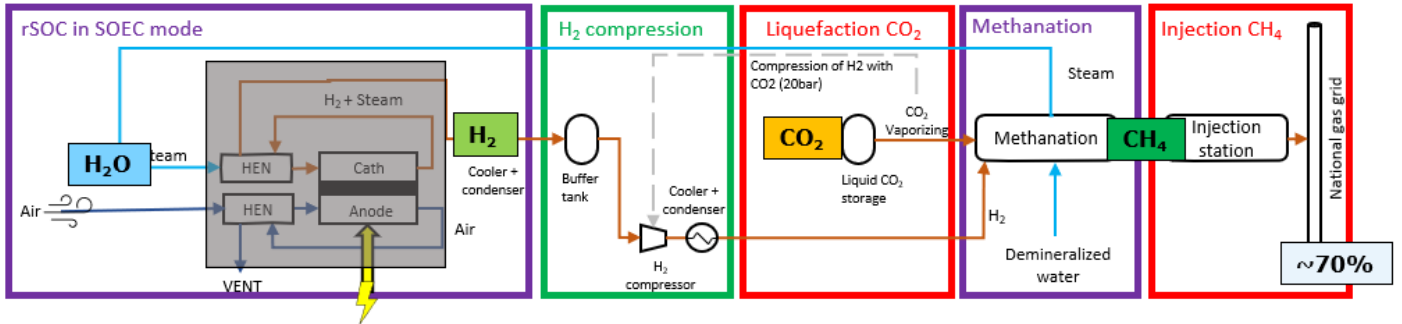
$$W_{comp,isot} = \left( \frac{10^5}{(3.6 \cdot 10^6)} \right) \cdot \left( \frac{p_1 v_1}{\eta_c} \right) \cdot \ln \left( \frac{p_2}{p_1} \right) \left[ \frac{kWh}{kg} \right]$$



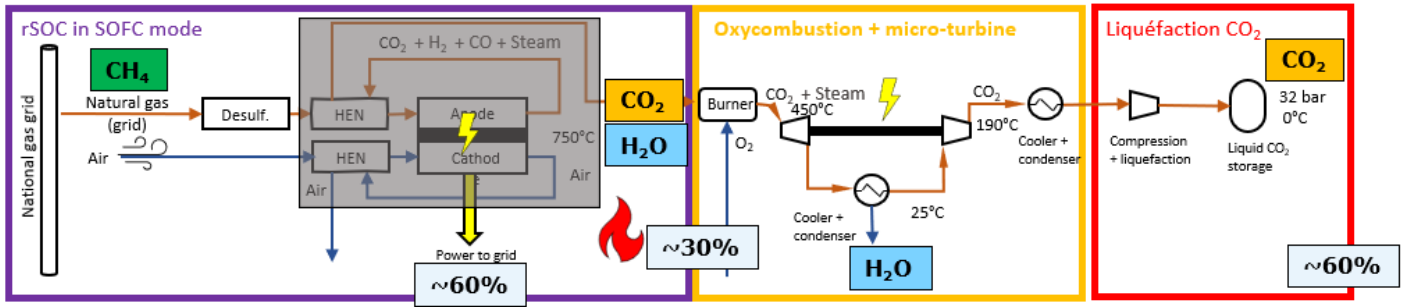
## Part 2

Consider a reversible solid oxide cell (rSOC) used for seasonal storage. During summer, as shown in the figure below, the rSOC is used as electrolyzer (SOEC) to produce H<sub>2</sub> from steam that is compressed and transferred into a methanator to produce methane by combining H<sub>2</sub> and CO<sub>2</sub>. The pressurized methane is then sent into the national gas grid. In winter the rSOC is used in fuel cell mode (SOFC) to produce electricity from the stored CH<sub>4</sub>. A micro gas turbine is coupled to the anode exhaust gas of the SOFC to produce even more electricity. The product, pure CO<sub>2</sub>, is easily stored by a simple compression process. The CO<sub>2</sub> is stored to be used for the methanation process during summer.

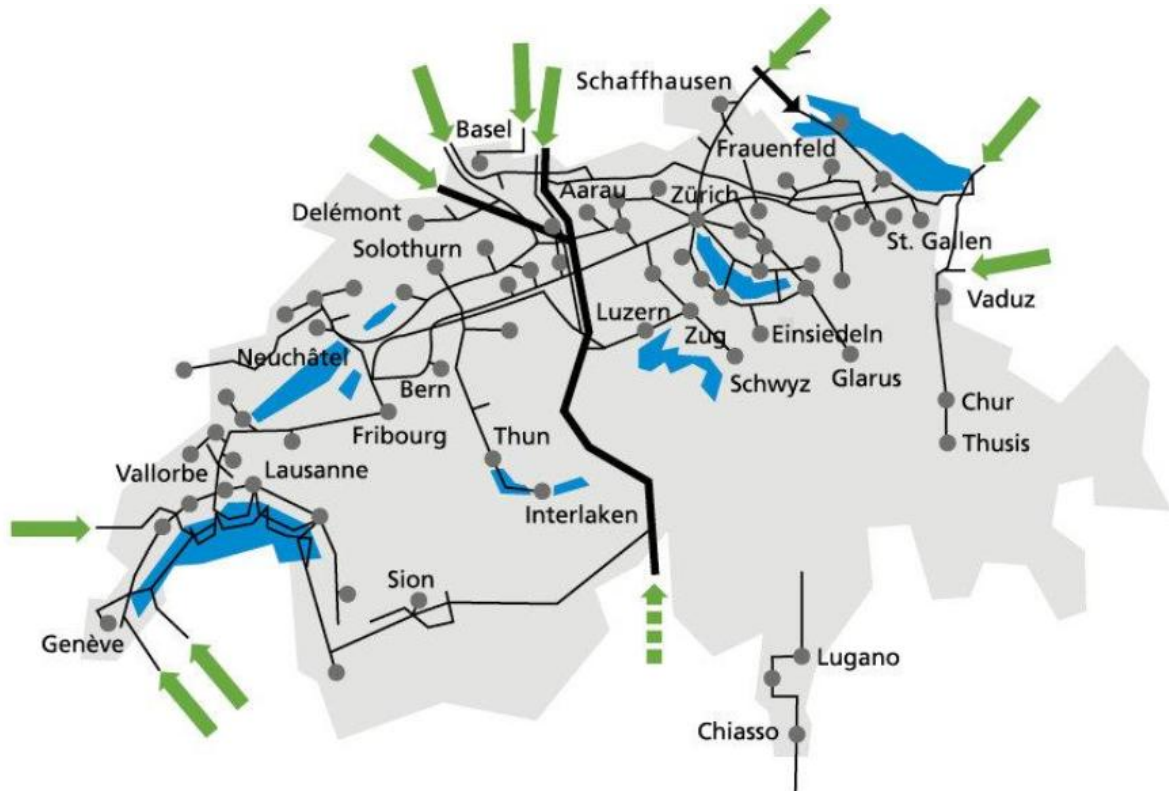
Summer



Winter



The solution of methane injection in a gas grid could be relatively easily implemented in countries where a national gas grid is well implemented such as Switzerland (figure below). It is not possible to transport hydrogen through the pipelines for the moment. The main gas grid is pressurized at 70 bar and made for methane. For industrial and local distribution, the pressure is lowered to 5 bar and for households the pressure is further lowered to a few mbar.



In winter, the SOFC is fueled with 0.96 kg/h of methane at atmospheric pressure, the electric output is 8.5 kW. The exhaust gases (remains of H<sub>2</sub> and CO) are burned in a catalytic burner with pure O<sub>2</sub> so that the combustion products are CO<sub>2</sub> and H<sub>2</sub>O. The heated gases are then expanded into the micro gas turbine which produces an electrical output of 0.7 kW. To account for the pumps, blowers, and losses, 0.5 kW is removed from this production. At the turbine outlet, pure CO<sub>2</sub> is compressed from atmospheric pressure to 35 bar and 0°C for storage as a liquid.

In summer, the fuel cell works in electrolyzer mode at 24 kW. The production is 0.7 kg/h of hydrogen. This hydrogen is compressed from 1 bar to 30 bar to enter the methanation part. The hydrogen is then combined with CO<sub>2</sub> to produce CH<sub>4</sub> and steam. The methanation process produces two flows, one of steam that is fueling the electrolyzer and the other flow is methane at 20 bar. The gas grid is set at 5 bar which means the expansion work from 30 to 5 bar could be recovered.

In case the methanation step is not included in the system, the produced hydrogen must be stored at a pressure of around 100 bar. To occupy less space, the pressure could be increased but at an important compression cost increase (specific volume of hydrogen = 11.12 m<sup>3</sup>/kg compared to methane at 1.39 m<sup>3</sup>/kg).

For the compression of CO<sub>2</sub>, we take reference from the values of Atlas Copco and the CO<sub>2</sub> booster CO<sub>2</sub> 2-195 – 50 that compresses CO<sub>2</sub> from 1 to 20 bar. The power consumption is found to be 0.173 kWh/kg.

- a) Compare this value with the adiabatic and isothermal compressions. What can you comment?

Pure adiabatic compression gives a value of 0.0977 kWh/kg and isothermal compression is 0.0674 kWh/kg. The compression is thus worst than the adiabatic compression, meaning that the efficiency of compression is relatively poor. This could be explained by the fact that the compression from 1 bar to 20 bar is made in a single stage, thus leading to large inefficiencies.

- b) Using the value of the CO<sub>2</sub> 2-195 – 50 booster, calculate the compression power required to compress a mass flow CO<sub>2</sub> = 2.86 kg/h from 1 to 35 bar.

$$P_{compr,CO_2} = W_{compr,manufacturer} \cdot \dot{m} = 0.5 \text{ kW}$$

- c) Find the system electric efficiency by performing the winter system energy balance assuming a mass flow of CO<sub>2</sub> = 2.86 kg/h and a low heating value of 50 MJ/kg for the methane.

$$\text{Power from CH}_4: 0.96 \text{ (kg/h}_{CH_4}) \cdot \text{LHV}_{CH_4} = 13.33 \text{ kW.}$$

Energy balance:

$$\eta_{winter} = \frac{P_{SOFC} + P_{mGT} - P_{compr,CO_2} - P_{loss}}{P_{CH_4}} = \frac{8.5 + 0.7 - 0.5 - 0.5}{13.33} = 0.615$$

$$= 61.5\%$$

During summer, we need to compress the produced H<sub>2</sub> from 1 to 20 bar. The multi-stage (5 stage) [ionic compressor IC 50/30-S](#) from Linde compresses hydrogen from 6 to 500 bar with a power consumption of 2.8 kWh/kg.

- d) Compare this value with the adiabatic and isothermal compressions. What can you comment?

Pure adiabatic compression gives a value of 4.3 kWh/kg and isothermal compression is 2.1 kWh/kg. The ionic compressor is thus closer to the isothermal compression which is good to reduce the compression cost. This was made possible by the multiple stage (5 stage) setup of the proposed compressor. This allows to cool down the stream between each stage.

Henceforth, we will assume the ratio between the manufacturers value and the adiabatic/isothermal compression to be constant.

$$xW_{(comp,adiab)} + (1 - x)W_{(comp,isot)} = W_{manufacturer} = constant \left[ \frac{kWh}{kg} \right]$$

- e) Using a mass flow of 0.7 kg/h, calculate the compression power for H<sub>2</sub> from 1 to 20 bar using the adiabatic and isothermal equations.

The ratio between the manufacturer's value and the adiabatic/isothermal curves is found to be 0.32.

$$P_{compr,H_2} = W_{comp} \cdot \dot{m} = 1.73 \cdot 0.7 = 1.21 \text{ kW}$$

- f) As the CO<sub>2</sub> is expanded from 35 bar to 20 bar and the produced methane is expanded from 20 to 5 bar with a respective mass flow of 4.45 kg/h and 1.72 kg/h, calculate the possible recovery power from these streams that could be used to partially compress the hydrogen.

$$P_{exp,CO_2} = W_{comp} \cdot \dot{m} = 0.0116 \cdot 4.45 = 0.052 \text{ kW}$$

$$P_{exp,CH_4} = W_{comp} \cdot \dot{m} = 0.07 \cdot 1.72 = 0.12 \text{ kW}$$

- g) Perform the summer system energy balance with a mass flow of CH<sub>4</sub> = 1.3 kg/h

Energy balance:

$$\eta_{summer} = \frac{P_{CH_4}}{P_{SOEC} + P_{compr,H_2} + P_{loss}} = \frac{18.1}{24 + 1.21 - 0.052 - 0.12 + 0.5} = 0.709$$

$$= 70.9\%$$

- h) Find the total round-trip efficiency

$$\eta_{round-trip} = \eta_{winter} * \eta_{summer} = 0.615 * 0.709 = 0.436 = 43.6\%$$

- i) In the case without the methanation part, hydrogen must be compressed to 100 bar. Calculate the new required compression power for hydrogen and comment.

$$P_{compr,H_2} = W_{comp} \cdot \dot{m} = 2.96 \cdot 0.7 \text{ kW} = 2.07 \text{ kW}$$

The compression power is 1.7 times greater with the methanation process. Taking this change and the fact that without the methanation process the supply of steam is no longer included inside the system, the round-trip efficiency will be negatively affected.