Hydrogen systems modeling

A brief introduction, mostly for control purposes

Robin Roche — robin.roche@femto-st.fr

FEMTO-ST, FCLAB, CNRS, Univ. Bourgogne Franche-Comte, UTBM

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Objectives of this lecture

- Briefly present the most common hydrogen technologies
- Explain how to select a model type
- Introduce reasonably simple stack models for these technologies
- Discuss system modeling and ageing-related issues
- List some related challenges

Outline

Outline

The big picture

In order to reach net zero emissions, (clean) hydrogen can help to:

- Massively integrate intermittent renewables
- Decarbonize transportation, heat, and industry

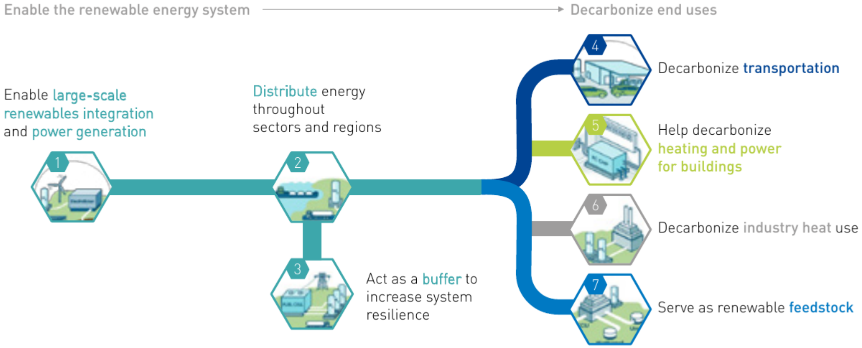


FIGURE 1 – Hydrogen as enabler of the energy transition in Europe (Source: fch.europa.eu)

This hydrogen can be produced, stored and consumed in different ways

Hydrogen technologies

In the following, we will focus on several hydrogen technologies:

- Electrolyzers, which produce hydrogen from water
- Tanks for storage in gaseous form
- Fuel cells, which enable generating electric power (and heat)

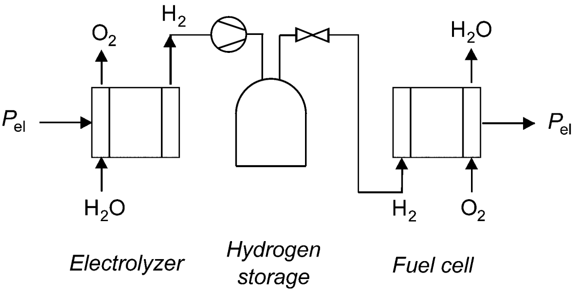


FIGURE 2 – Hydrogen energy storage principle (Source: 10.1039/C4EE04041D)

Other options, such as hydrogen combustion, will not be discussed here

Modeling hydrogen systems

As for many other fields, multiple models can be created for the same device

Simple models can be sufficient, while very detailed ones may be necessary

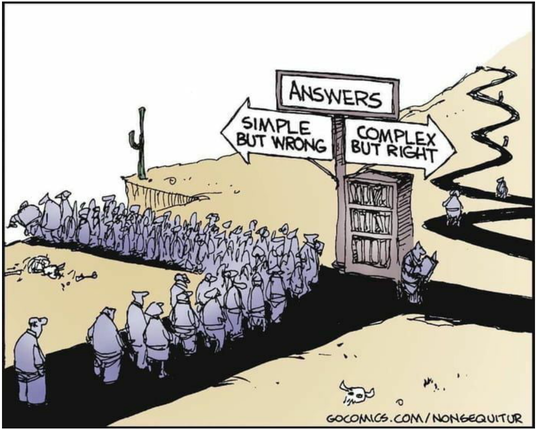


FIGURE 3 – simple vs. complex models (Source: gocomics.com)

Modeling hydrogen systems

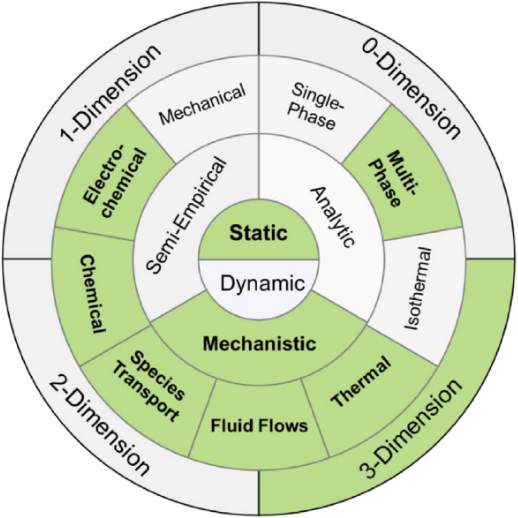


FIGURE 4 – Possible properties of hydrogen technologies models (Source: 10.1016/j.ijhydene.2021.02.170)

Modeling hydrogen systems

To decide on a model, different factors should be considered, such as:

- Time constants, from microseconds to seasons (see below)
- Accuracy requirements, limited by assumptions on input data
- Available calculation time and capacity

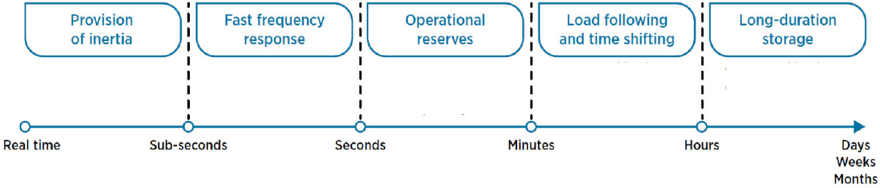


FIGURE 5 – Some services that can be provided by energy storage, including hydrogen (Source: irena.org)

Hydrogen can be used for a wide variety of applications:
use the most suitable model type depending on what is needed and possible

Let us now look at some of these models !

Outline

50 shades of hydrogen

Depending on how hydrogen is produced, different shades of hydrogen exist, e.g.:

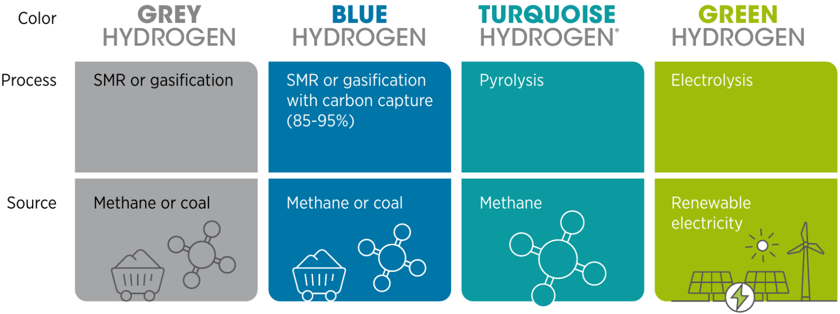


FIGURE 6 – The main shades of hydrogen (Source: irena.org)

About 95% is currently produced from fossil fuels: developing cleaner hydrogen water is therefore a priority !

Electrolysis principle

Discovered in 1800 by William Nicholson and Anthony Carlisle

Basic principle: split water (H_2O) into hydrogen (H_2) and oxygen (O_2)

Principle of operation:

- Non spontaneous transformation: needs an external energy source
- A DC current is passed through two **electrodes** placed in water
- An **oxidation** and a **reduction** enable to decompose water
- A separator or **membrane** separates both reactions and enables ions transfer
- **Stack** cells in series and parallel to increase voltage and current

For PEM technologies, we have the following reaction:

$$\begin{array}{llcl} \text{Anode (oxidation):} & 2\,H_2O_{(l)} & \rightarrow & O_{2\,(g)} + 4\,H^+ + 4\,e^- \\ \text{Cathode (reduction):} & 4\,H^+ + 4\,e^- & \rightarrow & 2\,H_{2\,(g)} \\ \hline \text{Overall reaction:} & 2\,H_2O_{(l)} & \rightarrow & 2\,H_{2\,(g)} + O_{2\,(g)} \end{array}$$

Electrolysis principle

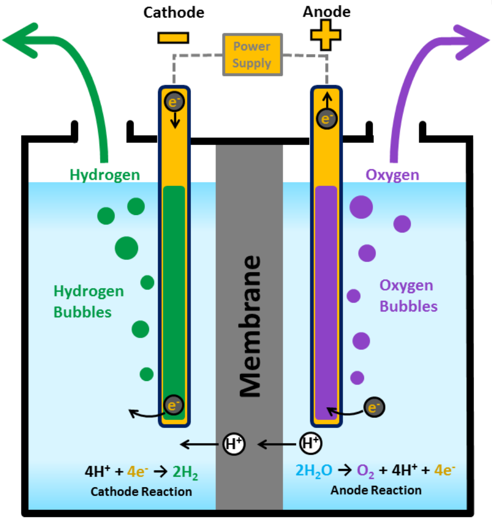


FIGURE 7 – Diagram of a PEM electrolyzer cell (Source: energy.gov)

Electrolyzer types

Although the overall reaction is the same, several types of electrolyzers exist and use different designs, e.g., for electrolytes and membranes / separators:

- **Alkaline** electrolyzers: mature, efficient
- **Proton exchange membrane (PEM)** electrolyzers: flexible, fast, compact
- **Solid oxide (SO)** electrolyzers: high temperature, in research

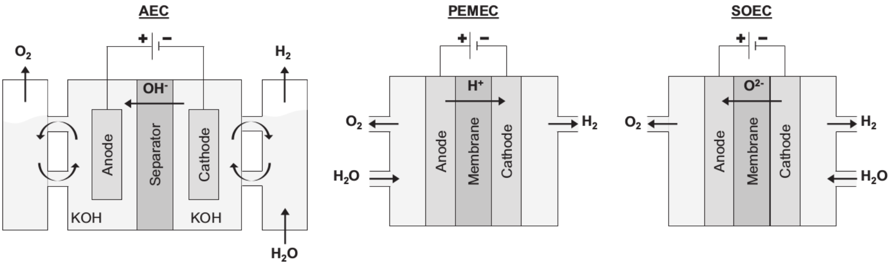


FIGURE 8 – Alkaline, PEM and SO electrolyzers (Source: 10.1016/j.ijhydene.2017.10.045)

In the following, we will focus on PEM technologies, as used in HAEOLUS

Electrolyzer KPIs

Performance and cost are crucial characteristics of electrolyzers

Some numbers according to IRENA in 2020, for MW-scale electrolyzers:

Type		Alkaline		PEM	
Indicators	Unit	**2020**	**2050**	**2020**	**2050**
Pressure	[bar]	<30	>70	<70	>70
Efficiency	[kWh/kg]	50-78	<45	50-83	<45
Lifetime	[kh]	60	100	50-80	100-120
Cold start	[min]	<50	<30	<20	<5
Capital costs (stack)	[USD/kW]	270	<100	400	<100
Capital costs (system)	[USD/kW]	500-1000	<200	700-1400	<200

TABLE 1 – Key performance indicators of electrolyzers in 2020 and 2050 (Source: irena.org)

Other KPIs of interest inlcude [14, 15]:

- Dynamic performance: ramping time, min. power, etc.
- Degradation, reliability, use of critical raw materials, etc.

Electrolyzer systems

Note that the stack is only a part of the system: multiple auxiliary parts, the balance of plant, are necessary to process input water and electricity, and output gases

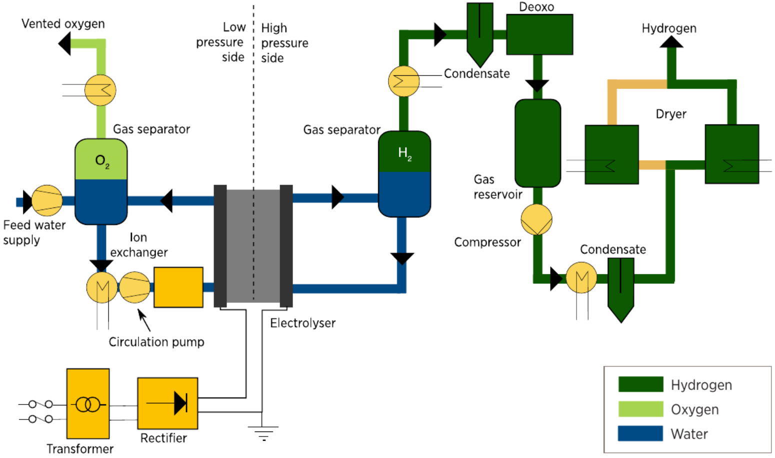


FIGURE 9 – Structure of a generic electrolyzer system (Source: irena.org)

Electrolyzer systems

FIGURE 10 – Picture of a 5 kW, 1 Nm^3/h, 33 cell, 50 bar PEM electrolyzer at UBFC

Electrolyzer systems

FIGURE 11 – Picture of a 1.2 MW PEM electrolyzer from Hydrogenics (now Cummins) used in the HyBalance project

Electrolyzer models

The simplest model is based on power and produced hydrogen [12]:

- The two equations below are generic
- Suitable applications: where only energy and/or power matter

$$P_{el}^{min} \leq P_{el}(t) \leq P_{el}^{max}$$

$$\dot{m}_{H_2,el}(t) = \eta_{el} \frac{P_{el}(t)}{HHV_{H_2}}$$

Var./param.	Description	Unit
P_{el}	Power consumption	[W]
η_{el}	System energy efficiency	–
HHV_{H_2}	Higher heating value	[J/kg]
$\dot{m}_{H_2,el}$	Produced hydrogen mass flow rate	[kg/s]

In reality, efficiency depends on the operation point, so such models are not very accurate and do not suit all applications

Electrolyzer models

For other applications such as short-term control or prognostics, more detailed models based on current and voltage may be necessary

Example of cell voltage or polarization curve and hydrogen flow rate model [13] :

Electrolyzer voltage : $$V = n_c \left(E_c + V_{act,c} + V_{act,a} + V_{ohm} + V_{diff} \right)$$

Open circuit voltage : $$E_c = E^0_{rev} + \frac{RT}{2F} \left(\ln \frac{p_{H_2} p^{1/2}_{O_2}}{p_{H_2O}} \right)$$

Activation overpotential : $$V_{act} = \frac{RT_a}{\alpha_a F} asinh \left(\frac{i}{2 i_{0,a}} \right) + \frac{RT_c}{\alpha_c F} asinh \left(\frac{i}{2 i_{0,c}} \right)$$

Ohmic losses : $$V_{ohm} = Ri$$

Mass transport overpotential : $$V_{diff} = \frac{RT}{nF} ln \left(\frac{C}{C_0} \right)$$

Hydrogen flow rate : $$\dot{m}_{H_2,el} = \eta_F \frac{n_c I}{2F}$$

Electrolyzer models

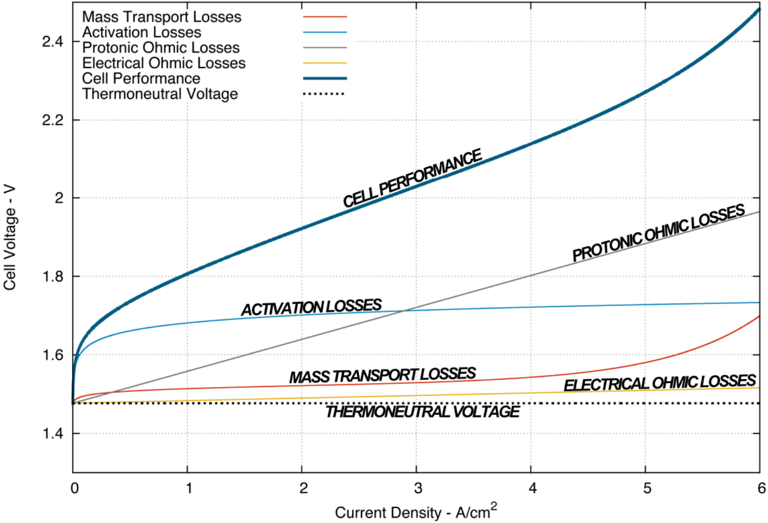
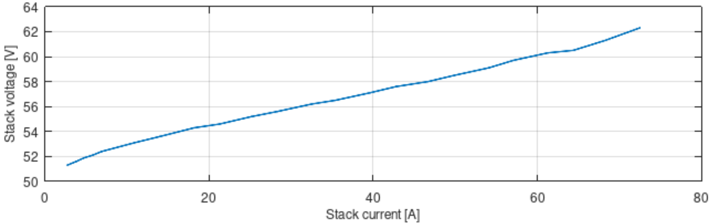


FIGURE 12 – Voltage of a PEM electrolyzer cell and breakdown of losses (Source: wikipedia.org)

Electrolyzer models

Example of experimental voltage curve for the 5 kW electrolyzer stack:



Modeling the rest of system requires considering various states:

State	Electrolyzer	Dryer	Approx. time
Standby	1.6 A	0.5 A	–
Deox warmup	–	4.5 A	10-20 min.
Purgeing during startup	9.0 A	–	–
Operation	27 A	0.7 A	–
Dryer column regenerating	–	4-7.5 A	120 min.
Shutdown	2.3 A	0.5 A	–

Outline

Overview of storage technologies

Hydrogen can be stored in various forms:

- Gas: mature, the most common form, with safety concerns
- Liquid: high density, but requires cooling to about 20 K
- Solid: not mature, high potential, complex heat management issues

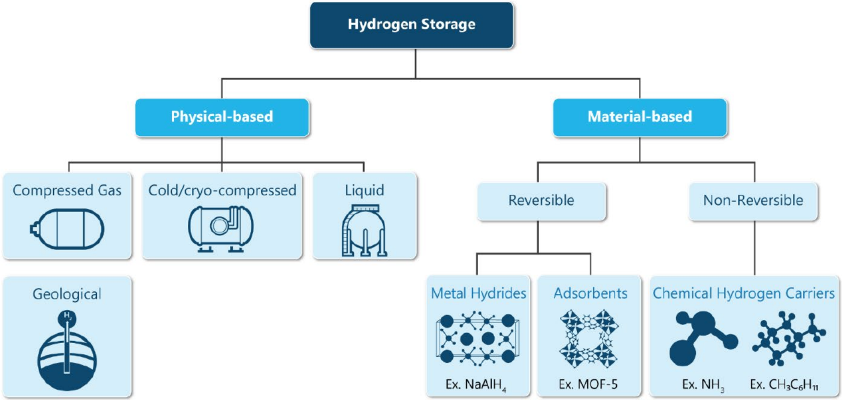


FIGURE 13 – Types of hydrogen storage technologies (Source: hydrogen.energy.gov)

A generic model

As for the electrolyzer, a generic model can be written as follows:

$$LOH(t) = LOH(t - \Delta t) + \frac{\Delta t}{m_{H_2}^{\max}} \left(\dot{m}_{H_2,el}(t) - \dot{m}_{H_2,fc}(t)\right)$$

$$LOH^{min} \leq LOH(t) \leq LOH^{max}$$

Var./param.	Description	Unit
LOH	Level-of-hydrogen	–
$m_{H_2}^{\max}$	Max. hydrogen mass	[kg]
Δt	Time step duration	[s]

This model suffers from several limitations, such as:

- Temperature has an effect
- Compression or conversion energy cannot always be neglected
- Pressure is usually the limiting factor for tanks

More detailed models are therefore necessary for some applications

Compressed gas storage

Why compress hydrogen ?

- High energy per unit mass, and a low energy per unit volume
- Storage volume is therefore a concern: a solution is to compress it
- Hydrogen is commonly stored in metal or composite tanks

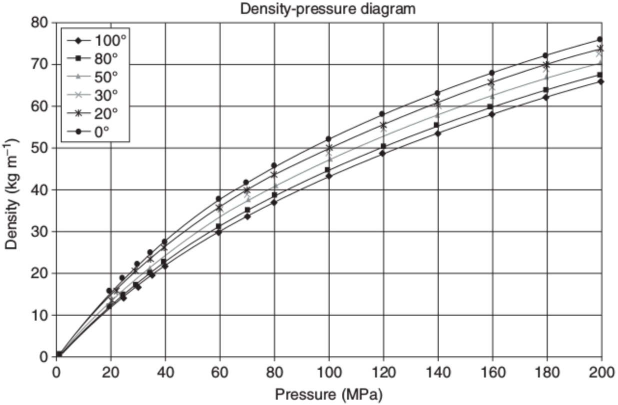


FIGURE 14 – Density of compressed hydrogen as a function of pressure and temperature (1 MPa = 10 bar) [7]

Compressed gas storage

Compressing gas does however impact efficiency, costs and reliability

Adiabatic compression work and power from p_0 to p_1 can be approximated by [16]:

$$W_c = \frac{\gamma}{\gamma - 1} R\, T \left[\left(\frac{p_1}{p_0} \right)^{\frac{\gamma-1}{\gamma}} - 1 \right]$$

$$P_c = \frac{1}{\eta_c} W_c\, \dot{m}_{el}$$

Var./param.	Description	Unit
W_c	Specific work	[J/mol]
γ	Ratio of specific heats	–
R	Universal gas constant	[J/mol·K]
T	Gas temperature	[K]
p_0, p_1	Initial, final pressure	[Pa]
η_c	Compressor efficiency	–
P_c	Compressor power	[W]

Compressed gas storage

Tank pressure is limited and given by a modified ideal gas law equation [3]:

$$p = Z\,\frac{nRT}{V}$$

Var./param.	Description	Unit
p	Gas pressure	[Pa]
Z	Compressibility factor	–
n	Number of moles	[mol]
R	Universal gas constant	[J/mol·K]
T	Gas temperature	[K]
V	Tank volume	[m^3]

The compressibility factor accounts for behavior at high pressure/temperature:

- Negligible at low pressure: $Z \approx 1$
- Non-negligible at high pressure: $Z > 1.1$ above 150 bar
- Determined experimentally

Compressed gas storage

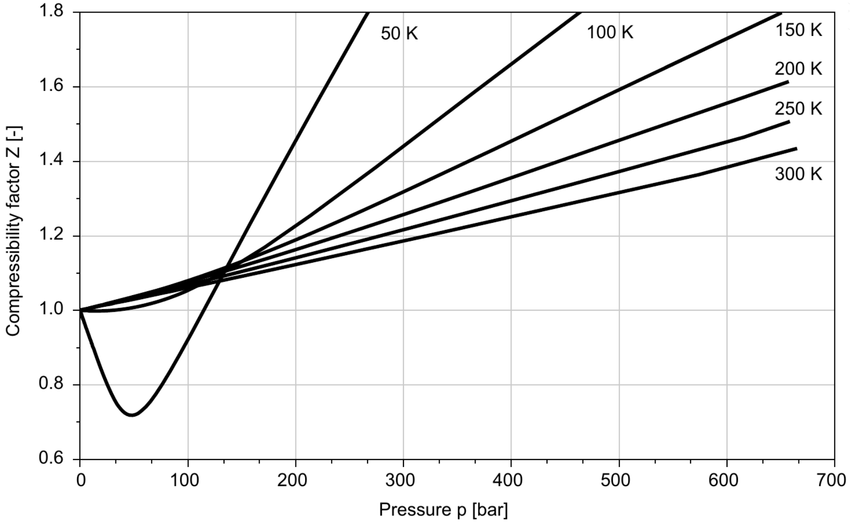


FIGURE 15 – Compressibility factor of hydrogen depending on temperature and pressure [3]

Compressed gas storage

Main characteristics of the steel tank used for HAEOLUS:

- Maximum operating pressure of 30 bar
- Volume of 64 m^3, which means a capacity of about 5 MWh

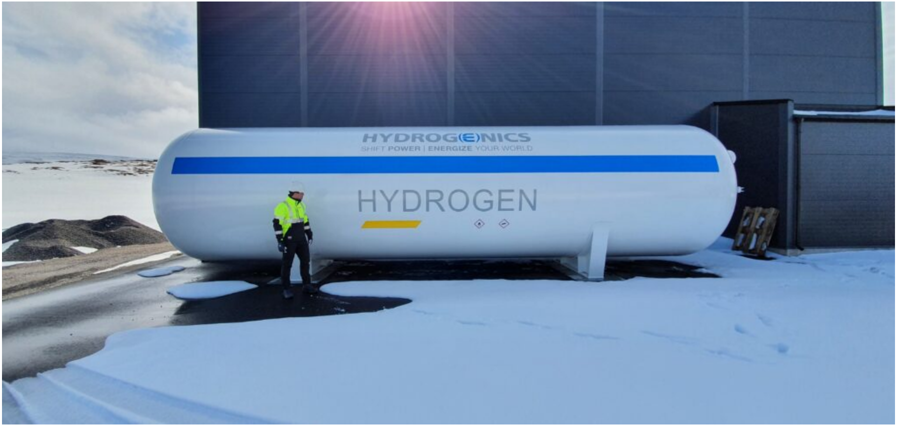


FIGURE 16 – Hydrogen storage tank used for demonstrator of the HAEOLUS project

Underground storage

An alternative to tanks is underground storage:

- Ideal for storing large (GWh) amounts of energy, e.g., in salt caverns
- Subject to multiple constraints: geology, availability, etc.

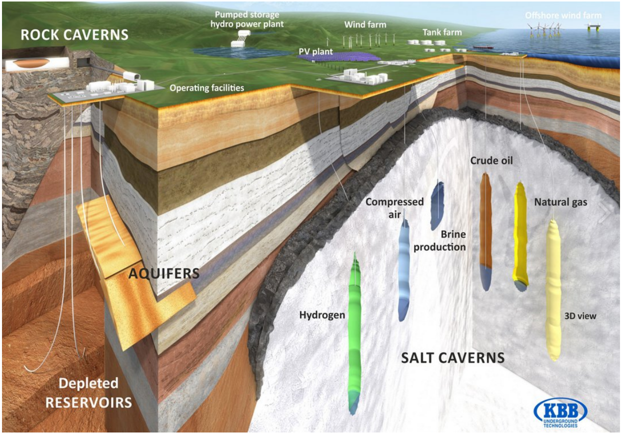


FIGURE 17 – Principle of underground gas storage (Source: forschung-energiespeicher.info)

Outline

Fuel cell principle

Invented in 1838 by William Grove, first modern applications in space in the 1960's

Basic principle:

- Generate electricity and water (H_2O) from hydrogen (H_2) and oxygen (O_2)
- So, somewhat the inverse of an electrolyzer... but this is not so simple in practice

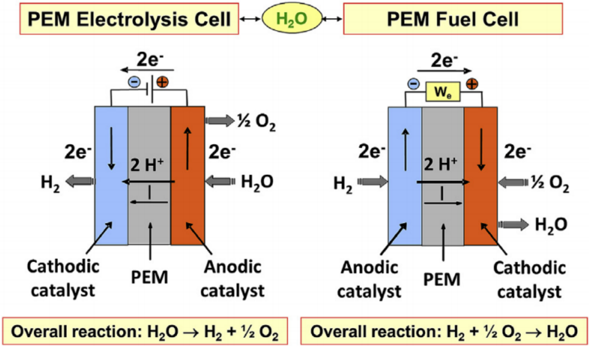


FIGURE 18 – Comparison of PEM electrolyzer and fuel cell schemes (Source: 10.1016/j.ijhydene.2016.04.173)

Fuel cell principle

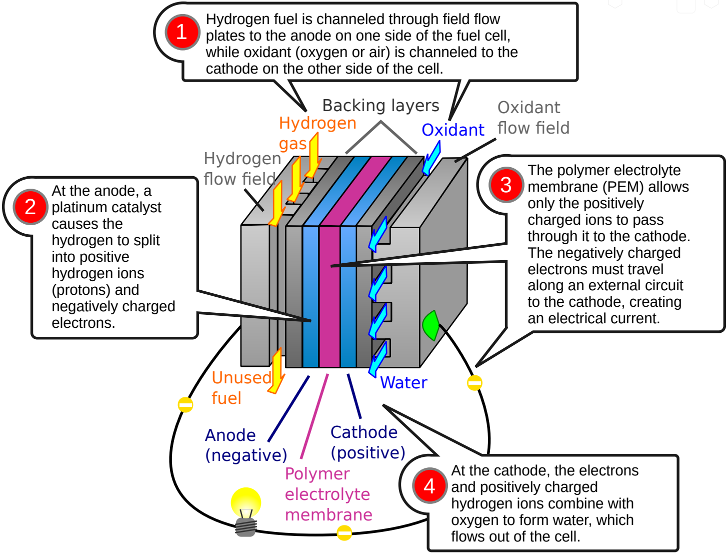


FIGURE 19 – Operation principle of a PEM fuel cell (Source: wikipedia.org)

Fuel cell principle

FIGURE 20 – A 500 W PEM fuel cell stack used for long duration tests at FCLAB

Fuel cell types

As for electrolyzers, there are several types of fuel cells, with different electrolytes, temperatures, charge carriers and applications:

- **Proton exchange membrane (PEMFC)**: low temperature, common for vehicles
- **Solid oxide (SOFC)**: high temperature, for cogeneration with heat reuse
- DMFC, AFC, PAFC, MCFC: less common, with specific challenges

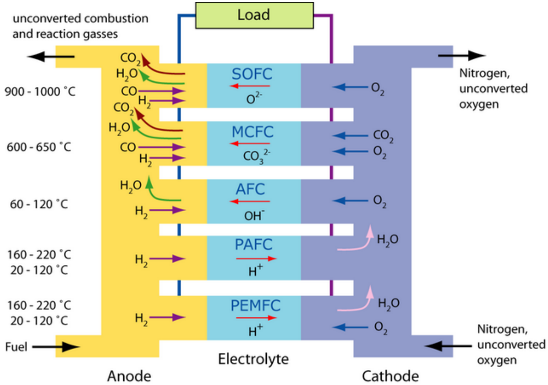


FIGURE 21 – A graphical comparison of the mechanisms of the different types of fuel cells (Source: doitpoms.ac.uk)

Fuel cell KPIs

As always, performance and costs are crucial criteria

Some recent and FCH-JU target numbers for **stationary** fuel cells according to [14]:

Indicators	Unit	**2017**	**2030**
Efficiency	% LHV	45	50
Reliability (MTTF)	[kh]	–	75
Lifetime (stack)	[kh]	20-60	25-60
Lifetime (plant)	[y]	15	25
Capital costs (stack)	[EUR/kW]	3000-3500	1200-1750

TABLE 2 – Key performance indicators of large (0.4–30 MW) stationary fuel cells for re-electrification in 2017 and 2030 [14]

Note that these numbers can be vastly different for other applications, e.g., in vehicles such as buses or trains where conditions can be more demanding

For example, the 2030 target for system lifetime in a bus is 28 kh

Fuel cell systems

As for electrolyzers, a number of auxiliary components are required to enable the fuel cell to operate: compressors, humidifiers, valves, electronics, cooling, etc.

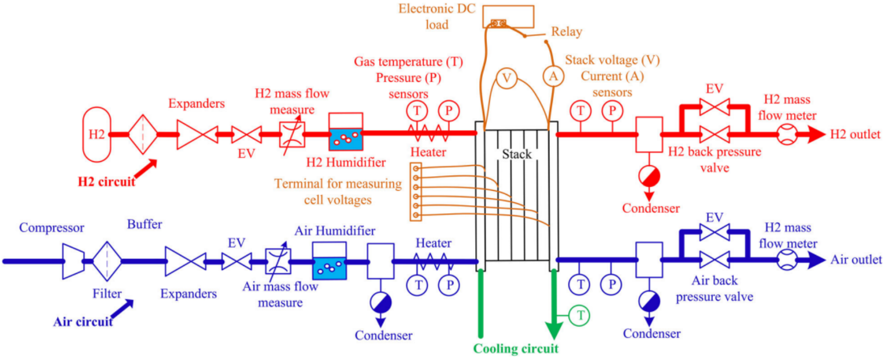


FIGURE 22 – Typical structure of a fuel cell test system (Source: 10.1186/s42500-019-0008-3)

These devices impact the system efficiency, reliability and costs: they are as important as the stack and should not be neglected

Fuel cell systems

Instrumentation is a key aspect to enable data acquisition and detailed modeling:

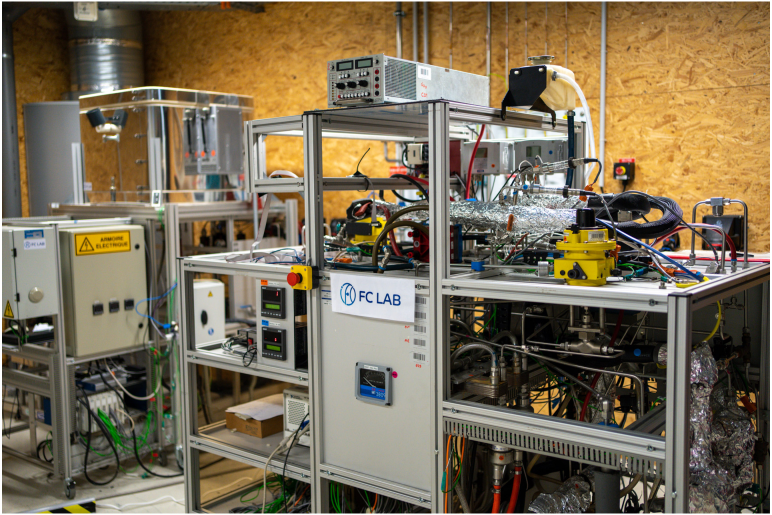


FIGURE 23 – A fully instrumented fuel cell test bench at FCLAB

Fuel cell systems

A commercial product example: Hydrogenics' HyPM HD 30 fuel cell

FIGURE 24 – A HyPM HD 30 (33 kW) fuel cell and balance of plant being installed for testing at FCLAB

Fuel cell models

As for electrolyzers, a generic and simplified model may be used:

$$P_{fc}^{min} \leq P_{fc}(t) \leq P_{fc}^{max}$$

$$\dot{m}_{H_2,fc}(t) = \frac{1}{\eta_{fc}} \frac{P_{fc}(t)}{LHV_{H_2}}$$

Var./param.	Description	Unit
P_{fc}	Fuel cell power output	[W]
η_{fc}	Fuel cell system efficiency	–
LHV_{H_2}	Lower heating value	[J/kg]
$\dot{m}_{H_2,fc}$	Consumed hydrogen mass flow rate	[kg/s]

This model is however unsuitable for many applications, where more advanced models, e.g., based on polarization curves, are necessary

Fuel cell models

This curve is similar to that of an electrolyzer, except that voltage decreases ; as a consequence, the power output of a stack peaks for a given current

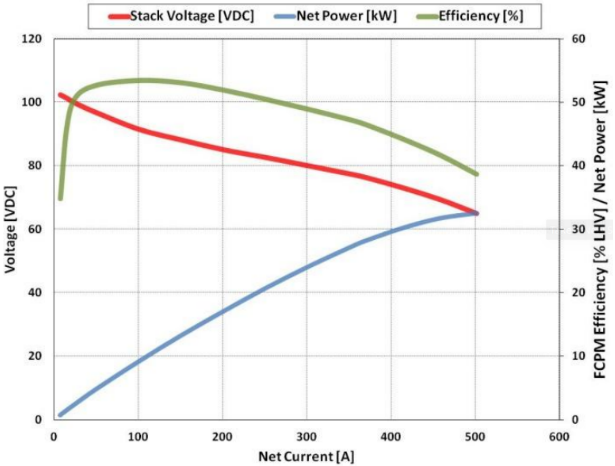


FIGURE 25 – Typical performance of a HyPM HD 30 fuel cell (from product datasheet)

Fuel cell models

Example of cell voltage or polarization curve and hydrogen flow rate model [2]:

Fuel cell voltage : $V = n_c\left(E_0 - V_{act} - V_{ohm} - V_{trans}\right)$

Open circuit voltage : $E_c = E^0 + \frac{RT}{2F}\left(\ln \frac{p_{H_2} p_{O_2}^{1/2}}{p_{H_2O}}\right)$

Activation losses : $V_{act} = A \ln\left(\frac{i + i_n}{i_0}\right)$

Ohmic losses : $V_{ohm} = ri$

Mass transport losses : $V_{trans} = -m \exp(ni)$

Hydrogen flow rate : $\dot{m}_{H_2,fc} = \frac{n_c I}{2F}$

This model is quite similar to that of the electrolyzer

Fuel cell ageing

Over time, components tend to degrade due to various phenomena, which impacts the voltage curve, and therefore the maximum power, but this is difficult to model

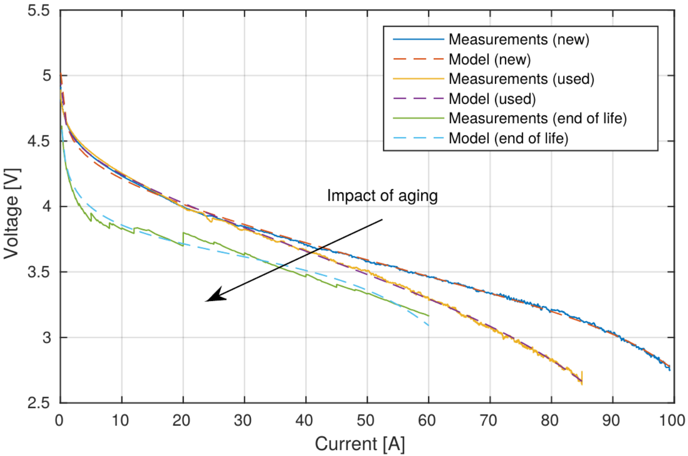


FIGURE 26 – Impact of operation duration (up to 2500 hours) on the voltage curve of a PEMFC (Source: 10.1109/ACCESS.2019.2930368)

Fuel cell ageing

Impedance spectroscopy is a tool which can be used to study the impact of various parameters on fuel cell performance and behavior

Accelerated stress tests can help facilitate such studies

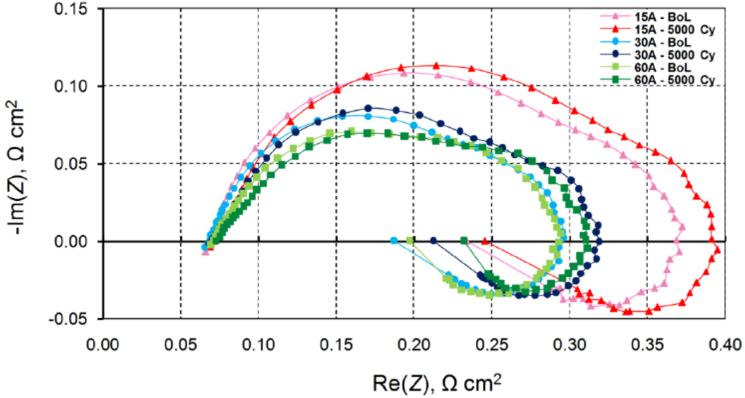


FIGURE 27 – Impedance spectra measured at beginning of life and after 5000 cycles of accelerated stress tests from the GIANTLEAP project (D1.4)

Outline

Conclusion

This lecture has given you a *brief* overview of selected hydrogen technologies and examples of easy to use models

Selecting the right model in is a tradeoff between accuracy and complexity which depends mainly on the considered application

The scope of modeling will also depend on the application:

- An embedded or islanded system will require modeling the balance of plant
- This could be neglected for a grid-connected application
- Sizing and control sometimes require modeling ageing and performance impacts

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For more information: femto-st.fr and fclab.org

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