

# Power-to-Gas Unit for Renewable Energy Storage

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In this work, dynamic modeling of Power-to-Gas work is presented. The created model was developed with Aspen Plus Dynamics™ tool. Required control strategies and additional Balance of Plant components were implemented to investigate Power-to-Gas transient behavior. Firstly, the developed model for Proton Exchange Membrane electrolysis went through a validation phase to highlight its performance regarding its ability to accurately describe the different phenomena observed in the real system. The created model was then scaled up to meet Electrolysis, Methanation and Oxy-combustion unit requirements. Given its ability to represent the entire system, its operation and its different dynamics, the developed model lends itself to different types of applications. In particular, a case study of coupling with wind farm entirely dedicated to synthetic natural gas production was analysed. The results of this integration have shown the ability of the developed concept to absorb electrical source intermittency. The observed limitations of this kind of application were underlined especially in the case of periods of low electricity production where a solution of buffer storage of excess hydrogen should be considered.

## 1. Introduction

The EMO unit (Electrolysis, Methanation and Oxy-combustion) is a concrete technological solution to the problem of intermittency of renewable energies and adapted to the evolution of energy needs in France in the medium and long term (2020-2050). Figure 1 shows the overall design of the EMO unit. Electric power is first converted to hydrogen in the proton exchange membrane (PEM) electrolyser. This hydrogen is reacted with carbon dioxide to form synthetic methane at the methanation process outlet. Oxygen co-produced by electrolysis as well as methane are stored in underground caverns. This is the Power-to-Gas phase of EMO unit. To recover stored energy, an oxy-combustion process is used to produce electricity as well as CO<sub>2</sub> which will be stored and reused in methanation process during the next cycle.

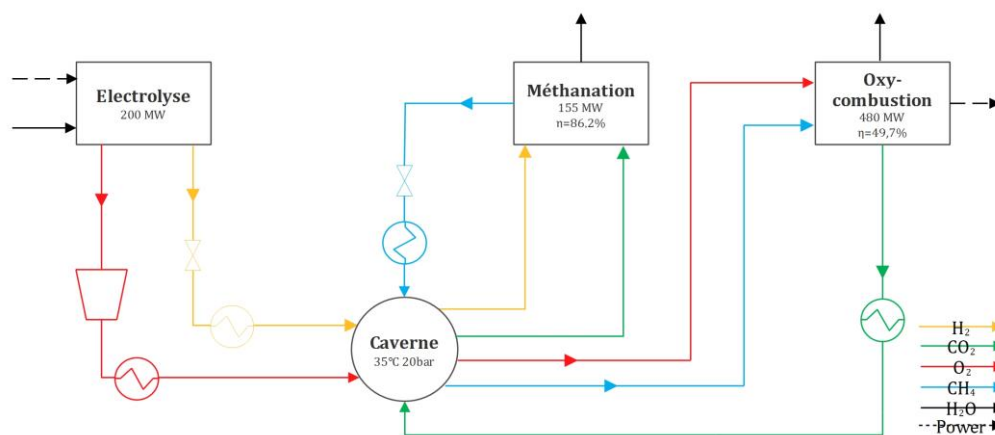


Figure 1: Overall layout of the EMO unit

Compared to conventional Power-to-Gas (PtG) processes, this new concept has two remarkable advantages; (i) it allows the use of oxygen co-produced by the electrolysis process and (ii) it ensures a continuous supply of carbon dioxide for the methanation unit. Both at PEM stack scale and PEM electrolyser system, the majority of models found in literature rarely include unsteady state operation. Some authors discussed the impact of fluid dynamics on stack (Görgün, 2006) or system level (Nie et al., 2009). In the work of Grigoriev et al. (2010), the conducted analysis deals with: (i) calculation of the output flow of the stack in order to establish mass balance at each electrode; (ii) calculating the level in the separators; (iii) impact of the flow of water circulation on the behavior of bubbles and their evacuation or (iv) CFD modelling of flow characteristics at bipolar plates. More recently, Er-rbib et al. (2017) investigated one of the most emerging technologies of electricity conversion: reversible solid oxide cells (RSOC) and Er-rbib et al. (2018) assessed the performance of a power-to-gas process based on this technology. Oliver et al. (2017) were among the rare authors to develop a multiphysics model for a complete PEM electrolysis system. The aim was to identify the dynamic behaviour of the technology for Power-to-Gas applications (i.e. coupling with renewable energy sources). Their model uses the Bond Graph formalism to represent the electrolyser stack as well as the rest of the auxiliary components conventionally found in a commercial machine. The Bond Graph formalism, which follows a modular configuration, was found to be flexible enough to allow structural or sensitivity analysis of system parameters. Dynamic model of PEM electrolyser system

## 2. Dynamic model of PEM electrolyser system

### 2.1 Reference PEM electrolysis system

The steady state model of PEM electrolyser was used as a basis for the development of the dynamic model using Aspen Plus Dynamics™ tool. The equations used to describe the electrochemical, thermal and kinetic phenomena that occur within PEM stack have been modified to take into account unsteady state operation. This includes material and energy balance as described by the equations Eq(1)-Eq(7):

$$\text{Anode} \quad H_2O \quad \frac{dn_{H_2O,an}}{dt} = \dot{N}_{H_2O,in,an} - \dot{N}_{H_2O,out,an} - \dot{N}_{H_2O,m} - \dot{N}_{H_2O,cons} \quad (1)$$

$$H_2 \quad \frac{dn_{H_2,an}}{dt} = \dot{N}_{H_2,in,an} - \dot{N}_{H_2,out,an} + \dot{N}_{H_2,m} \quad (2)$$

$$O_2 \quad \frac{dn_{O_2,an}}{dt} = \dot{N}_{O_2,in,an} - \dot{N}_{O_2,out,an} + \dot{N}_{O_2,prod} - \dot{N}_{O_2,m} \quad (3)$$

$$\text{Cathode} \quad H_2O \quad \frac{dn_{H_2O,ca}}{dt} = \dot{N}_{H_2O,in,ca} - \dot{N}_{H_2O,out,ca} + \dot{N}_{H_2O,m} \quad (4)$$

$$H_2 \quad \frac{dn_{H_2,ca}}{dt} = \dot{N}_{H_2,in,ca} - \dot{N}_{H_2,out,ca} + \dot{N}_{H_2,prod} - \dot{N}_{H_2,m} \quad (5)$$

$$O_2 \quad \frac{dn_{O_2,ca}}{dt} = \dot{N}_{O_2,in,ca} - \dot{N}_{O_2,out,ca} + \dot{N}_{O_2,m} \quad (6)$$

$$\text{Energy Balance} \quad C_{th} \frac{dT_{in,an}}{dt} = (T_{out,an} - T_{in,an}) \sum C_p i \dot{N}_{i,out}^{an} - \dot{W}_{el} + \dot{N}_{H_2,prod} \Delta H_r \quad (7)$$

Where  $\dot{n}$  (mol.s<sup>-1</sup>.m<sup>-2</sup>),  $\dot{N}$  (mol.s<sup>-1</sup>), T (K), W (W) correspond to molar flow rate density, species molar flow rate, temperature and power and *an*, *ca*, *el*, *prod* correspond to the indexes relating to anode side cathode side, electric and production.

During the transition from steady state to dynamic state models, several components have been added to ensure system control under transient conditions. In particular, PID controllers were added to regulate separator tanks pressures. On-off controllers were also used to regulate stack temperature and tanks levels. These regulators parameters were chosen to adequately represent experimental data retrieved from the test rig (Kezibri, 2018). A model validation step was then to compare the results of the dynamic model with the experimental data from the test rig. This comparison was performed under rated power conditions.

### 2.2 EMO unit electrolysis module

Using the previously developed architecture for the 10 MW<sub>t</sub> electrolyser module (Kezibri and Bouallou, 2017), a dynamic model was created for the scaled-up process to characterise its behaviour during different transient

phases. Figure 2 shows the flowsheet of the developed model. Unlike steady state model, the system is completed by the addition of a pure water tank (WT) as well as system required regulation for pressures, temperatures and tank levels.

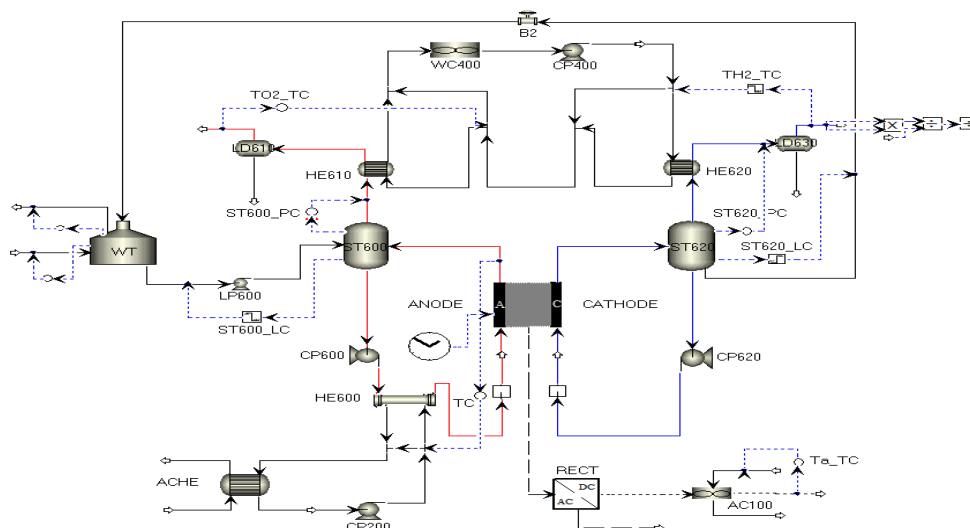


Figure 2: Dynamic Model of PEM electrolyser module (system control in dashed blue lines)

The analysis will focus on the flexibility of the system and its ability to follow load changes through the monitoring of its main characteristics. This also includes the measurement of load change impact system overall efficiency and purity of produced gases.

In the studied process, the dimensioning of the auxiliary equipment is as necessary as reactor sizing to provide an accurate dynamic response of the overall system. Particularly, this work has focused on the main components of the heat recovery network (i.e. steam cycle). The heat exchangers are sized based on process rated performance. Aspen Exchanger Design™ tool was used to size all seven heat exchangers using a shell and tube design. This sizing allows an accurate calculation for heat transfer performance as well as pressure drop estimation.

In order to allow a more realistic behaviour of the steam cycle performance, performance curves for each of the used turbines and circulation pumps are integrated. The model will re-evaluate the cycle's performance with each undergone change by means of specific work and isentropic efficiencies.

### 3. Results

This part is dedicated to a case study of a scenario that approaches a real operation of the installation. A renewable electricity production from a wind farm dedicated entirely to energy storage is considered. The quantities of hydrogen and SNG (Synthetic Natural Gas) that can be produced depending on load profiles intermittency at Power-to-Gas system are analysed.

#### 3.1 Wind energy production

To generate power production profiles of the considered wind farm, the open-source SAM (System Advisor Model) tool developed by the US national renewable energy laboratory NREL is used. This simple tool allows the prediction of wind farm annual production by means of real meteorological data. The model takes into account the influence of several physical quantities measured for the simulated periods and usually provided on hourly basis. These parameters include wind speed and direction as well as air temperature and pressure at given altitude.

The wind farm was chosen to have a total installed power of 300 MW<sub>e</sub> which is slightly higher than overall electrolysis process consumption of the EMO unit at rated power. In this case study, the wind farm consists of 100 Vestas V90 wind turbines of 3 MW<sub>e</sub> each. Based on these input data, SAM tool simulates hourly production of the wind farm over one-year period. This result is used to select two representative periods of wind energy production seasonality. February was considered for winter season with a total electricity production of 120 GWh and August for summer period with a total electricity production of 65 GWh. Based on these assumptions, summer period of the year is characterised by a strong discontinuity of electricity production (Figure 3). The duration of production periods is relatively short, often below 24 h. The wind farm runs at rated capacity for only

a few hours in this period. On the other hand, winter period is relatively more favourable to wind generation. It is characterised by longer production durations and more frequent rated power operation of the wind farm.

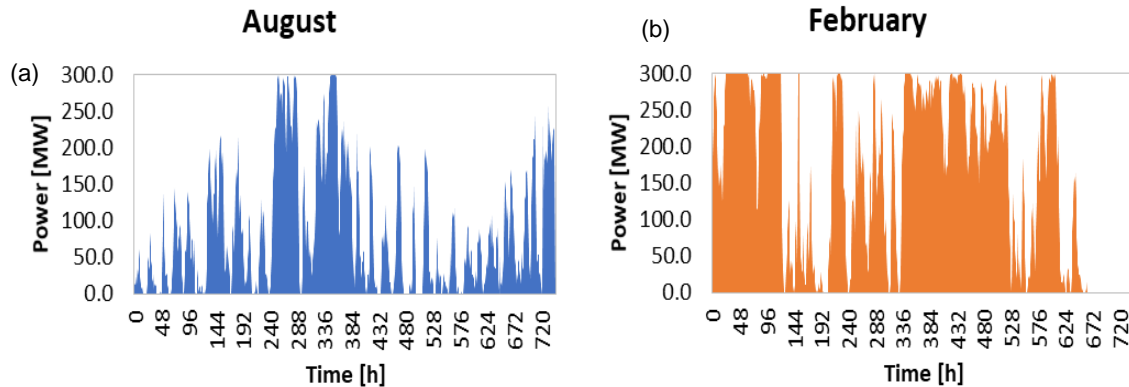


Figure 3: Hourly generated wind power for (a) August and (b) February

### 3.2 Coupling with Power-to-Gas process

The PEM electrolysis process and CO<sub>2</sub> methanation dynamic models were combined to simulate the production of hydrogen and SNG based on available power at the wind farm output.

In this approach, an equivalence between each PEM electrolyser module of EMO unit was assumed. The power available at system input is equitably distributed over the 20 modules available forming the electrolysis process. With the results of dynamic analysis in mind, range operation of each module is restricted to 2 % of rated power. When this limit is reached, the electrolyser system is switched to stand-by mode where operating current density is set to zero.

Regarding methanation process, limitations defined through unsteady state analysis are taken into account. In particular, a feed stream of reactants at stoichiometric proportion was assumed. This assumes continuous availability of carbon dioxide from underground storage. The process operating range is set between 48 % and 100 % of rated power. This range, demonstrated in the previous subsection, firstly allows to maintain acceptable temperatures for proper operation of fixed bed reactors (i.e. between 250 and 600 °C.). It also produces an SNG with at least 95 % methane molar fraction. It guarantees steam quality at both turbines inlets in the cogeneration cycle. By analysing the respective electrical production curves for each month, periods that are favourable for SNG production given electrical power availability and process limitations have been identified. These periods are summarised in Table 1.

Table 1: Results of SNG production for chosen periods

Period	Start	End	Duration [h]	Produced SNG [GWh]	Consumed H <sub>2</sub> [GWh]	Consumed CO <sub>2</sub> [t]	Backup H <sub>2</sub> [Nm <sup>3</sup> ]
August	130	159	29	2.77	3.61	499	36,275
	245	292	47	6.58	8.46	1,169	0
	322	385	63	7.81	10.1	1,396	3,385
	726	744	18	2.24	2.87	397	0
<b>Total</b>	–	–	<b>157</b>	<b>19.4</b>	<b>25.0</b>	<b>3,461</b>	<b>39,660</b>
February	0	122	122	17.4	22.6	3,737	5,426
	212	235	23	3.39	34.0	4,699	0
	336	524	188	26.3	7.13	985	0
	575	616	41	5.53	4.39	607	0
<b>Total</b>	–	–	<b>374</b>	<b>52.6</b>	<b>68.1</b>	<b>10,028</b>	<b>5,426</b>

Potential periods of operation requiring high hydrogen backup were excluded. These periods would require massive hydrogen storage capacities which is not intended for the EMO unit primary design. For the summer period (August), the production of 19.4 GWh of synthetic methane requires more than 3,461 t CO<sub>2</sub>, which corresponds to around 21 operational hours of the oxy-combustion cycle at rated power. The winter period

(February) consumes up to 10,028 t CO<sub>2</sub> to produce 52.6 GWh of synthetic methane, equivalent to running the oxy-combustion cycle for about 57 hours.

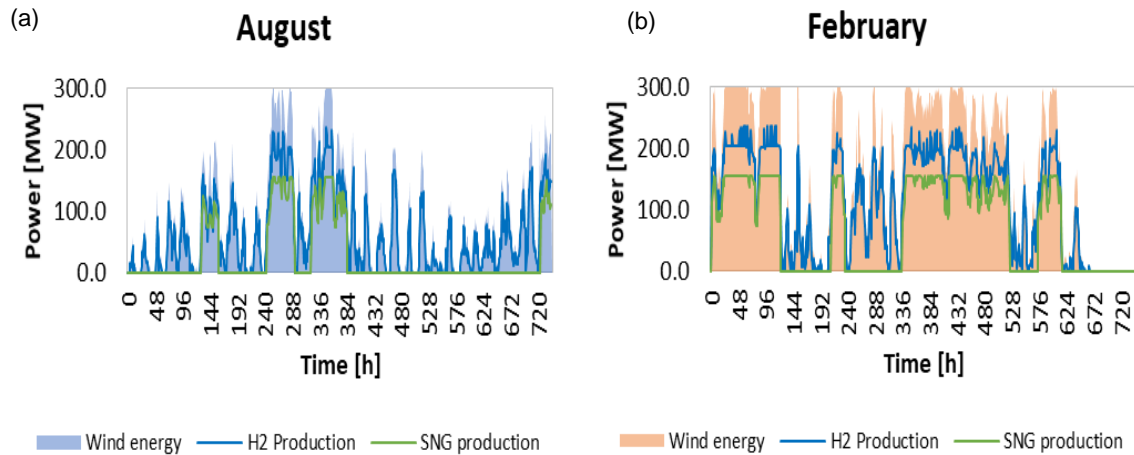


Figure 4: Simulation of (a) hydrogen and (b) SNG production from wind power for chosen periods

The simulation results of wind farm coupling with Power-to-Gas process indicate (Figure 4) that a maximal production of 46.1 GWh of hydrogen is possible in summer period, compared to 84.0 GWh in winter. Given the operational limitations of methanation process, only 54.2 % of this hydrogen is consumed by the reactors to produce 19.4 GWh of SNG in summer, compared to 81.0 % in winter, to produce 52.6 GWh of SNG. In this specific case, it would be more efficient for periods with low renewable electricity generation, to consider underground storage for excess hydrogen production.

The simulation results are used to analyse energy efficiency of Power-to-Gas process for the two considered periods. This efficiency combines the performances of both PEM electrolysis and carbon dioxide methanation processes. Overall, process efficiency stays close to the rated value of 57.4 %<sub>HHV</sub>. During winter period, this value appears in a more frequent and consistent manner compared to summer period. This fluctuation is also linked to the initial assumption which considers a uniform distribution of inlet electric power to all PEM electrolysis modules. However, by optimising electricity distribution across these modules, a lower efficiency operation that can occur during limited electric power availability can be avoided.

To conclude this case study, the results obtained for hydrogen and SNG production in August and February are applied to the rest of the year. Firstly, a summer production period starting from May to September which will follow the same production performance observed for August has been defined. The second winter period, from October to April, will follow the typical production performance of February. The basic assumption here is to consider that each month of summer period can convert 71.0 % of available wind power into hydrogen and 29.9 % of that same power into SNG. Similarly, each month of winter period can convert 70.3% of renewable electricity into hydrogen and 43.9 % into SNG. These ratios are retrieved from the characteristic performance of each respective period shown in Sankey diagrams (Figure 5).

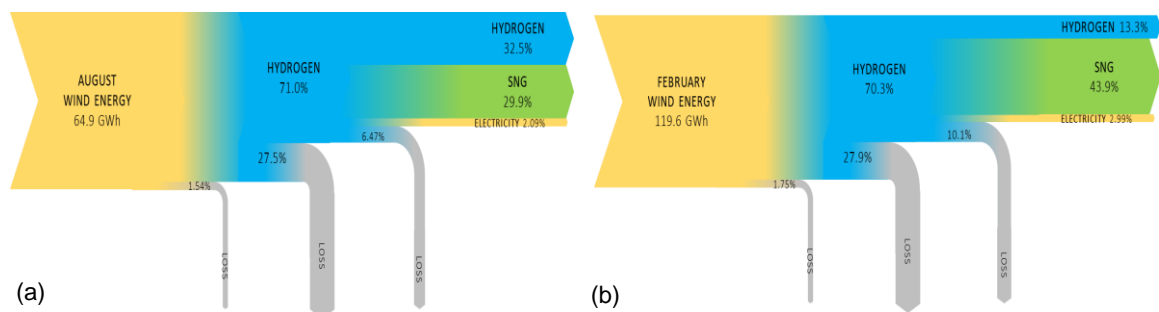


Figure 5: Sankey diagrams of Power-to-Gas performance during (a) summer and (b) winter periods

The annual production of hydrogen and SNG based on specific performance of each characteristic period can be estimated. Figure 6 shows the result of this analysis applied to one year of wind farm production. From 1,219 GWh of renewable electricity produced by the 300 MW wind farm, the PEM electrolysis process is able to produce up to 859 GWh of hydrogen, which represents 70.4 % of total input energy. On the other hand, the Power-to-Gas process is able to produce up to 488 GWh per year of SNG, representing 40.0 % of the annual electrical energy supplied by the wind farm. This production of synthetic methane will require about 91,752 t carbon dioxide, equivalent to an annual operating time of 560 h for the oxy-combustion process.

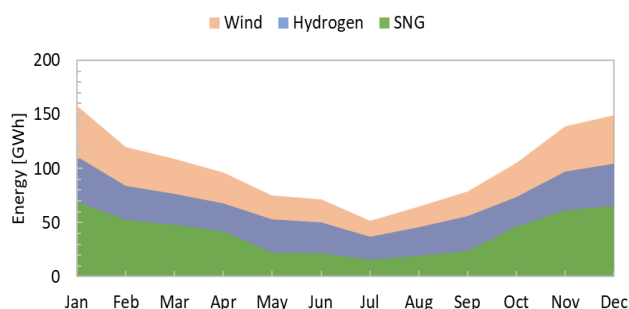


Figure 6: Prediction of monthly production of hydrogen and SNG from wind energy

#### 4. Conclusion

In this work, dynamic modelling of Power-to-Gas work was presented. The created model was developed with Aspen Plus Dynamics™ tool. Required control strategies and additional Balance of Plant components were implemented to investigate Power-to-Gas transient behaviour. Firstly, the developed model for PEM electrolysis went through a validation phase to highlight its performance regarding its ability to accurately describe the different phenomena observed in the real system. The created model was scaled up to meet EMO unit requirements. Given its ability to represent the entire system, its operation and its different dynamics, the developed model lends itself to different types of applications. In particular, a case study of coupling with wind farm entirely dedicated to SNG production was analysed. The results of this integration has shown the ability of the developed concept to absorb electrical source intermittency. Observed limitations of this kind of application were underlined. Especially in the case of periods of low electricity production where a solution of buffer storage of excess hydrogen should be considered.

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