



Intelligent electroFuel production for An Integrated STorage System

Deliverable 3.1

Report on the development and validation of the model

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Executive summary

The deliverable summarizes the results from tasks “T3.2 - Development of detailed mathematical models and implementation in the Matlab environment” and “T3.3 - Validation of the models by comparison with the results of the monitoring”, the goal of which was to develop and validate a dynamic physics-based model of a Power-to-Gas system (PtG) for the production of synthetic methane. The research group of the University of Parma has developed an in-house library of models for integrated energy systems which serves to build their digital twins, i.e. models that emulate the behavior of the real system with high-detail and typically faster than real-time. Each block represents a physical component that can be found in multi-energy networks, covering various domains, i.e. heat, electrical energy, fuels. The aim, features and governing equations of the sub-models of the components are described with specific reference to the elements of the case study: the wind farm, the PtG system (electrolyzer, methanation, condenser), the gas storages, the district heating circuit (pumping station, pipelines, heat exchangers), as well as the heat pump and the boiler. The library has shown to be a reliable tool for accurate simulations of distribution networks with different energy domains. Thus, a digital twin of the system considered was built by combining together the components from the library. The multi-energy system simulated consists of a wind farm which produces electricity, that can be used to fulfill the electrical needs of the end-user or can be used by a PtG system for the production of synthetic methane. The waste heat of the PtG plant is recovered using an Heat Recovery Circuit (HRC), which works at low-temperature level: then, it is upgraded to the temperature level needed by a district heating network (DHN) through an Heat Pump and it is used, together with a gas-fueled boiler, to fulfill the thermal needs of the end-user through a district heating network.

The digital twin is significantly faster than real time, reliable and useful for several purposes. It can be simulated for long periods, and it will be exploited as a virtual testbed for verifying a novel management strategy based on Model Predictive Control.

1 Introduction

This report is the deliverable D3.1 of work package WP3 of the IFAISTOS project, which is led by the University of Parma. The work package "WP3 - System modeling and control" aims at develop a system model of a Power-to-Gas (PtG) system for the production of synthetic methane, and an optimization algorithm suitable for its optimal management within a Model Predictive Controller. The deliverable summarizes the results from tasks "T3.2 - Development of detailed mathematical models and implementation in the Matlab environment" and "T3.3 - Validation of the models by comparison with the results of the monitoring", the scope of which was to develop and validate a dynamic physics-based model of a PtG system for the production of synthetic methane. The proposed model is built by assembling in a coherent way the models of the single energy systems that constitute it, which represent a library of components developed in Matlab®/Simulink® environment by the research group of the University of Parma. It collects the most common components that can be found in integrated energy networks.

2 Library of energy systems

A detailed nonlinear model, which emulates the real system, was developed in the MATLAB®/Simulink® environment, and it was built by assembling the models of single energy system components. The application consists of a wind farm, a PtG system for the production of synthetic methane (electrolyzer, methanation reactor and condenser), an Heat Recovery Circuit (HRC) which recovers the waste heat from the PtG system exothermic components, an Heat Pump (HP) which upgrades the temperature level of the recovered heat, a gas-fueled boiler and a District Heating Network (DHN), which ensures heat supply to an end-user.

The Simulink® library used to model the DHN was already presented in previous works [1], and it is composed by pumping station (expansion vessels and pumps), heating network (pipelines) and thermal power units (boilers and heat exchangers). Nevertheless, for the present application, new components were developed, that constitute the PtG plant [2]. The main components and how they were modeled is presented below.

2.1 Wind farm

This is an algebraic model that, starting from the undisturbed wind velocity module and direction u_0 , and given the geometry of the wind turbines and their position in the wind farm, calculates the output electrical power production. The electrical power produced by each turbine is calculated starting from the power curve, given the wind velocity. For a wind farm with N wind turbines, the total electrical power generated is calculated as

$$P_{el} = \sum_{i=1}^N C_p(u_{w,i}) P_{w,i} = \sum_{i=1}^N C_p(u_{w,i}) A_{r,i} \rho u_{w,i} \quad (1)$$

where $P_{w,i}$ is the wind power reaching the i -th turbine of the wind farm, $A_{r,i}$ is the area of the i -th turbine rotor, ρ is the air density and $C_p(u_{w,i})$ is the power coefficient with a wind velocity equal to $u_{w,i}$, which is the velocity of the wind reaching the i -th turbine, corrected considering the wake effect. Indeed, when considering a wind farm with multiple turbines, the model considers the wake effect by applying the Jensen wake model. With this method, the wake effect is taken into account by applying a correction to the undisturbed wind velocity, when the turbine is located behind other turbines in the wind direction. The corrected wind velocity $u_{w,i}$ for each turbine i is calculated starting from the undisturbed wind velocity u_0 as follows

$$u_{w,i} = u_0 - u_{mdef,i} = u_0 - \sqrt{\sum_{j=1}^N u_{def,ij}} \quad (2)$$

where, the velocity deficit $u_{def,ij}$ caused by the upstream turbine j on the downstream turbine i is calculated as

$$u_{def,ij} = u_0 (1 - \sqrt{1 - C_{t,j}}) \left(\frac{D_{r,i}}{D_{r,i} + 2k_{w,i}x_{ij}} \right)^2 \frac{A_{overlap,ij}}{A_{r,i}} \quad (3)$$

where $D_{r,i}$ is the downstream turbine rotor diameter, $C_{t,j}$ is the thrust coefficient of the upstream turbine, $k_{w,i}$ determines the size of the expanded wake behind the wind turbine, x_{ij} is the distance between the two turbines in the wind direction and $A_{overlap}$ is the overlap area between the expanded wake area of the upstream wind turbine and the rotor area of the downstream turbine $A_{r,i}$. Once the corrected wind velocity $u_{w,i}$ for each turbine is determined, the power curve of the turbines is used to calculate the electricity generated.

2.2 PEM electrolyzer

The model of the electrolyzer is an algebraic model that, given the electrical power supplied and the operating mode returns the amount of hydrogen and the thermal power generated. It has three different operating mode: ON, OFF (i.e. no consumption, no production, cold start-up needed to switch on), standby (i.e. no production, consumption of a certain amount of nominal electrical power, warm start-up needed to switch on). During the steady state operation, the relation for the efficiency of the electrolyzer is derived by interpolating operating data, as shown in Figure 1. The relationship obtained from data in Figure 1 is the following

$$\eta = \rho H H V \frac{a P_{el}^b + c}{P_{el}}, \quad (4)$$

and it is used to calculate the hydrogen flow rate produced as follows

$$\dot{V}_{H_2} = \frac{1}{\rho H H V} \eta P_{el}, \quad (5)$$

with ρ being the gas density, HHV its high heating value and P_{el} the input electric power. The thermal power generated is calculated using the following equation

$$P_{th} = (1 - \eta)P_{el} - P_{loss}, \quad (6)$$

where P_{loss} represents the non-recoverable heat and it is calculated as $P_{loss} = \alpha P_{nom} + (\beta P_{el} + \gamma P_{nom})$: the first term represents the losses due to the auxiliary systems, while the latter terms represent the linear model of the power losses in the conversion from AC to DC.

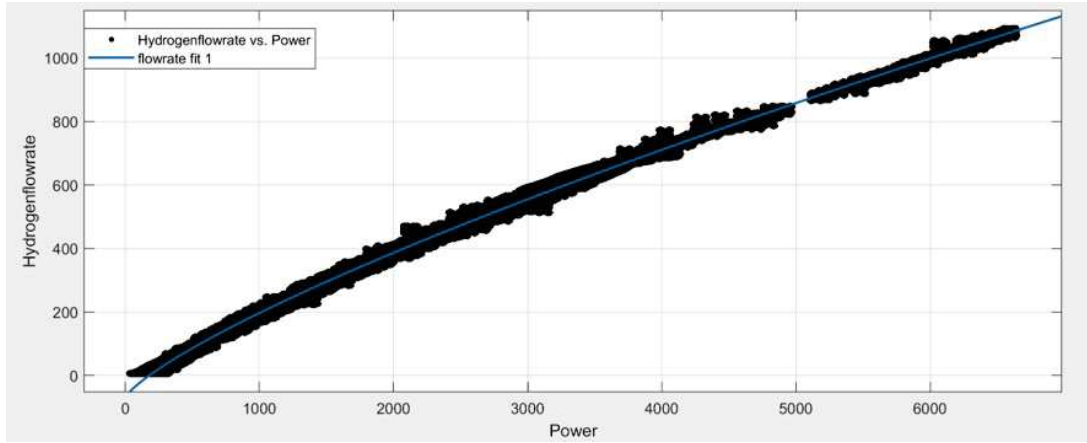
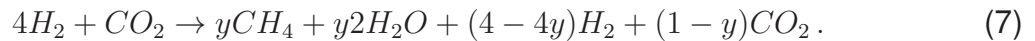


Figure 1: Data used for the identification procedure for the calculation of output hydrogen flow rate from the electrolyzer (black dots), taken from [3], and fitting obtained, i.e. Eq (4) (blue line).

2.3 Methanation reactor

This is an algebraic model that correlates the input hydrogen flow to the output methane flow and thermal power generated. Similarly to the electrolyzer, it has three operating modes: ON, OFF and standby. In the steady state operation, the output flow is calculated using the yield of reaction y , with the chemical reaction



The yield of reaction y is calculated based on linear interpolation of experimental data, as shown in Figure 2, with the following relationship

$$y = a \frac{GHSV}{GHSV_{nom}} + b, \quad (8)$$

where GHSV (gas hourly space velocity) is the rate between the total volumetric flow rate at inlet and the reactor volume, and evaluates the load of the reactor:

$$GHSV = \frac{\dot{m}_{H_2,in} + \dot{m}_{CO_2,in}}{V_{reactor}}. \quad (9)$$

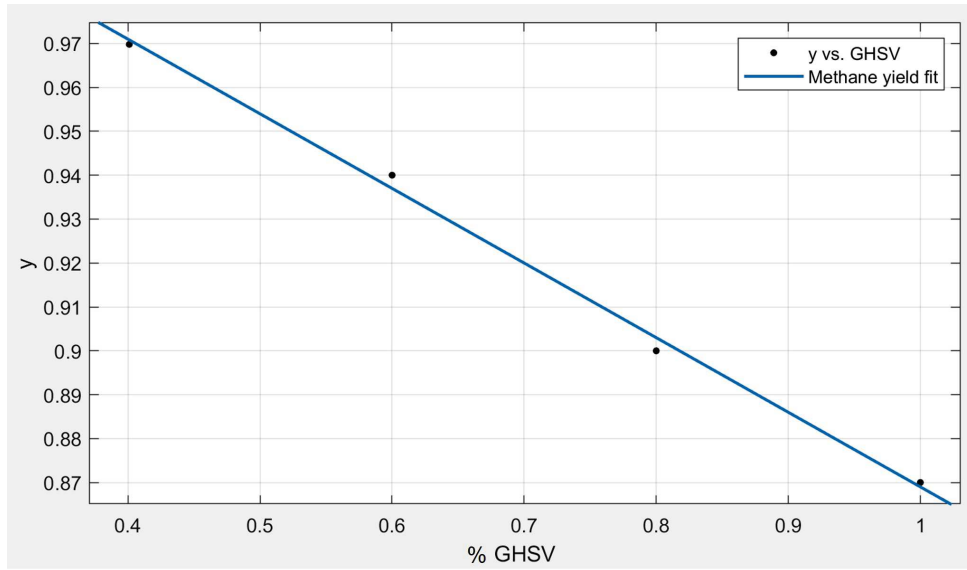


Figure 2: Data used for the identification procedure for the calculation of the methanator yield (black dots), taken from [4], and fitting obtained, i.e. Eq (8) (blue line).

2.4 Gas compressor

The compressor model is an algebraic model that, given the rotational speed, the input flow and the output desired pressure, calculates the output flow and the electrical power consumption. The block contains the performance maps of turbocompressor for the calculation of the corrected mass flow rate \dot{m} (Figure 3) and of the polytropic efficiency η_p (Figure 4), given the corrected rotational speed N_c and the pressure ratio β . Since no data were available for that operating region, the corrected mass flow rate and the polytropic efficiency have been considered constant in the choking area.

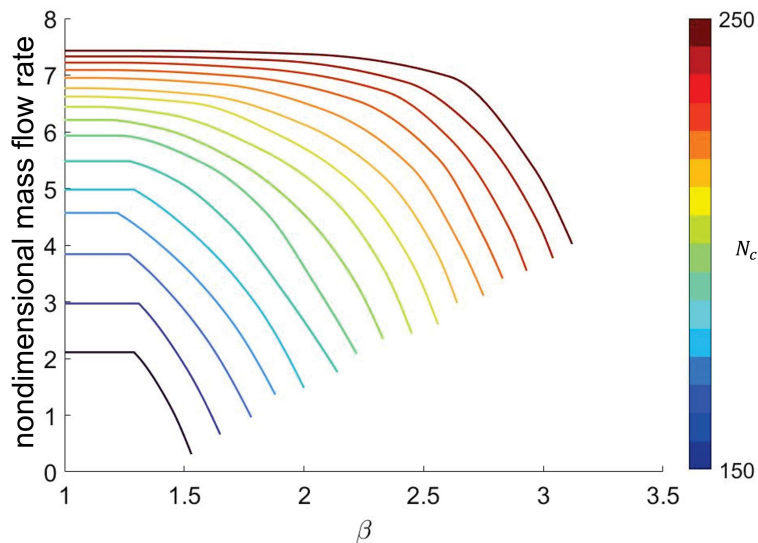


Figure 3: Turbocompressor performance map for mass flow rate.

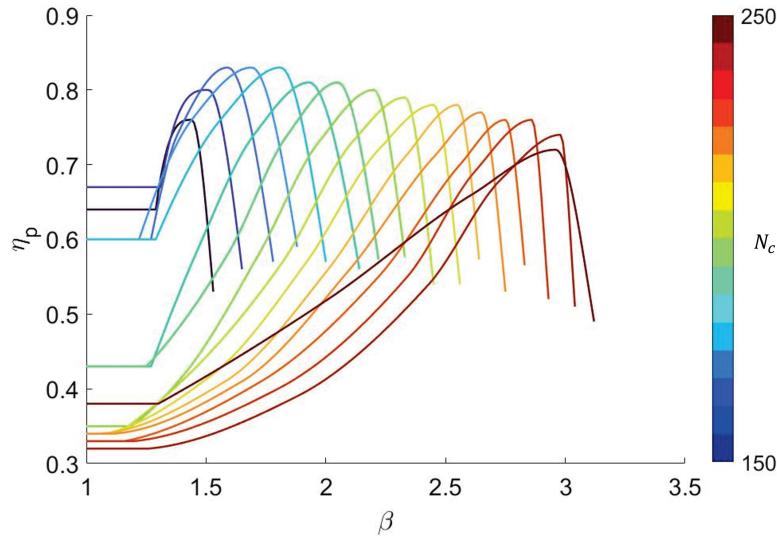


Figure 4: Turbocompressor performance map for polytropic efficiency.

2.5 Gas storage

The proposed model represents a node in which the input flow is mixed with the gas inside the storage. It is a dynamic model that uses the energy balance and continuity equations for pressure and temperature calculation. In terms of causality, incoming and outgoing flows are known, and the model calculates the pressure, temperature and composition of the gas contained in the storage. The energy stored is calculated using the gas HHV.

Gases are described through the perfect gas equation of state. The mass balance equation for gases allows the calculation of the mass and molar composition of gases present in the volume:

$$\frac{dm_g}{dt} = \dot{m}_{g,in} - \dot{m}_{g,out} , \quad (10)$$

and the energy balance equation for gases allows to calculate the temperature of the gases

$$\frac{dT_g}{dt} = \frac{\Delta\dot{H}_g - c_v T_g \frac{dm_g}{dt} - m_g T_g \sum_i \frac{\partial c_v}{\partial w_i} \frac{dw_i}{dt}}{c_v m_g + m_g T_g \frac{\partial c_v}{\partial T}} , \quad (11)$$

where c_v is the specific heat of the gas at constant volume, w_i is the mass fraction of the i -th gas species and $\Delta\dot{H}_g$ is the power linked to the enthalpy flows of the gas phase species and it is calculated as

$$\Delta\dot{H}_g = \dot{H}_{g,in} - \dot{H}_{g,out} = [(\dot{m}_g c_p T)_{in} - (\dot{m}_g c_p T)_{out}] . \quad (12)$$

The partial pressure for each species is calculated as

$$p_i = \frac{m_i RT}{M_i V} . \quad (13)$$

2.6 Water condenser

It is a dynamic model that, starting from the incoming and outgoing flows, calculates the pressure, temperature, amount of water condensed and composition of the gas exiting the condenser. A wet mixture enters the condenser, it is cooled and therefore the steam condenses by accumulating liquid water at the base of the discharger. When the water reaches a certain level, the drain opens and the water flows out in a liquid state. The dry gas mixture is taken from another outlet.

The mass and energy balance equation, the perfect gas equation of state and the law of Antoine, which allows to calculate the saturation pressure of water, are used in the model. The mass balance equation for gases allows to calculate the mass and molar composition of gases present in the volume:

$$\frac{dm_g}{dt} = \dot{m}_{g,in} - \dot{m}_{g,out} - \dot{m}_{H_2O,cond}, \quad (14)$$

the mass balance equation for liquid water allows to calculate the volume, at the base of the steam trap, occupied by the condensed water:

$$\frac{dm_{h_2O}}{dt} = \dot{m}_{H_2O,cond} - \dot{m}_{H_2O,out}, \quad (15)$$

and the energy balance equation for gases allows to calculate the temperature of the gases in the condensate discharger:

$$\frac{dT_g}{dt} = \frac{\Delta\dot{H}_g - \dot{H}_{H_2O} - P - \dot{Q}_{sc} - c_v T_g \frac{dm_g}{dt} - m_g T_g \sum_i \frac{\partial c_v}{\partial w_i} \frac{dw_i}{dt}}{c_v m_g + m_g T_g \frac{\partial c_v}{\partial T}}, \quad (16)$$

where w_i is the mass fraction of the i -th gas species, P is the power due to the work related to the volume change

$$P = p \frac{dV_g}{dt}, \quad (17)$$

and $\Delta\dot{H}_g$ is the power linked to the enthalpy flows of the gas phase species and it is calculated as

$$\Delta\dot{H}_g = \dot{H}_{g,in} - \dot{H}_{g,out} = \dot{m}_g [(c_p T)_{in} - (c_p T)_{out}] + \dot{m}_{cond} r_v + [(\dot{m}_v c_p T)_{in} - (\dot{m}_v c_p T)_{out}]. \quad (18)$$

Finally, to determine the water steam flow rate that condenses, the saturation pressure value of water is used, using the Antoine's law

$$\log_{10} p_s = A - \frac{B}{T + C}, \quad (19)$$

where A, B, C are constants, obtained experimentally and T is the temperature in Celsius. The partial pressure for each species is calculated as

$$\frac{dp_i}{dt} = \frac{RT}{M_i V} \sum_i \dot{m}_i - \frac{p_i}{V} \frac{dV}{dt} + \frac{p_i}{T} \frac{dT}{dt}. \quad (20)$$

2.7 Gas pipeline

This is a dynamic model that, given the inlet pressure, temperature and composition, and the outlet pressure, calculates the output mass flow rate and temperature of the gas. The mass flow rate is calculated as follows

$$\dot{m} = \text{sign}(\Delta p) \sqrt{\frac{|\Delta p| \rho A_{cs}}{\frac{\lambda L}{D_{in}} + Z}}, \quad (21)$$

where Δp is the pressure drop in the pipeline, A_{cs} is the cross-section area of the pipeline, ρ is the gas density, λ is the friction factor, L is the pipe length, D_{in} is the inner diameter, Z represents the total concentrated pressure drop. The governing equation for the temperature is the following

$$\frac{dT_{out}}{dt} = \frac{1}{\rho c_v V} \left(\dot{m} \left[(c_p T)_{in} - (c_p T)_{out} \right] - \dot{Q}_w \right), \quad (22)$$

where c_p is the gas specific heat at constant pressure, c_v is the average gas specific heat at constant volume, V is the volume of the pipeline and \dot{Q}_w is the heat exchanged through the wall.

2.8 Heat pump

This is an algebraic model in which the thermal power absorbed and supplied by the heat pump are calculated based on the temperature of the cold and hot sources (T_c and T_h) and on the electrical power used P_{el} . The actual COP is calculated as follows

$$COP = \frac{COP_{nom}}{C_c(1 - (1 - C_c))} \frac{P_{el,nom}}{P_{el}}, \quad (23)$$

where C_c is a correction factor usually declared by the manufacturer, $COP_{nom} = \frac{COP_{max}}{\eta_{II}}$ and η_{II} is the second principle efficiency and it is calculated with a lookup table with $\eta_{II} = f(T_c, T_h)$.

2.9 Gas pressure reduction valve

The gas pressure reduction valve model is an algebraic model that takes as inputs the income and outcome pressure, temperature and composition of the gas, and opening ratio of the valve, and returns the mass flow rate through the valve. The mass flow rate is calculated using the expansion factor Y , which is calculated as

$$Y = 1 - \frac{1}{3} \left(\frac{x}{F_k x_T} \right), \quad (24)$$

where

$$x = \frac{\Delta p}{p_{in}}, \quad (25)$$

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F_k is the ratio between the k of the gas and the k of air $F_k = k/k_{air}$ and x_T is the value of x when Y reaches its minimum value ($Y = 2/3$).

Then, if $\frac{2}{3} \leq Y \leq 1$, namely when the gas is in sub-critical conditions, the mass flow rate is calculated as

$$\dot{m} = N_x c_v Y \sqrt{x p_{in} \rho_{in}}, \quad (26)$$

where N_x is a coefficient introduced to match the measurement units used. When $Y = \frac{2}{3}$, instead, the fluid is in super-critical conditions and, being $x = x_T$, the mass flow rate equation becomes

$$\dot{m} = N_x c_v \frac{2}{3} \sqrt{x_T p_{in} \rho_{in}}. \quad (27)$$

The inputs, outputs and states of all the components are reported in Table 1, for pumping station, heating network and thermal power units the details are reported in [1].

Component	AI/Dy	Inputs	Outputs	States	Main governing equations
Wind farm	AI	\mathbf{u}_{wind}	P_{el}	-	$P_{el} = \sum_{i=1}^N C_p(u_{w,i}) P_{w,i}$ $\sum_{i=1}^N C_p(u_{w,i}) A_{r,i} \rho u_{w,i}$ $u_{w,i} = u_0 - u_{mdef,i} = u_0 - \sqrt{\sum_{j=1}^N u_{def,ij}}$ $u_{def,ij} = u_0 \left(1 - \sqrt{1 - C_{t,j}}\right) \left(\frac{D_{r,i}}{D_{r,i} + 2k_{w,i} x_{ij}}\right)^2 \frac{A_{overlap}}{A_{r,i}}$
Electrolyzer	AI	P_{el} Op mode	$\dot{m}_{out}, T_{out}, x_{out}, p_{out}$ $\dot{m}_{H_2O}, P_{th}, P_{loss}$	-	$\eta = \rho HHV \frac{aP_{el}^b + c}{P_{el}}$ $\dot{V}_{H_2} = \frac{1}{\rho HHV} \eta P_{el}$ $P_{th} = (1 - \eta) P_{el} - P_{loss}$
Methanation reactor	AI	$\dot{m}_{in}, T_{in}, x_{in}$ Op mode	$\dot{m}_{out}, T_{out}, x_{out}$ P_{th}, P_{loss}	-	$4H_2 + CO_2 \rightarrow yCH_4 + y2H_2O + (4 - 4y)H_2 + (1 - y)CO_2$ $y = a \frac{GHSV}{GHSV_{nom}} + b$ $GHSV = \frac{\dot{m}_{H_2,in} + \dot{m}_{CO_2,in}}{V_{reactor}}$
Gas compressor	AI	$N,$ $p_{in}, p_{out}, T_{in}, x_{in}$	$\dot{m}, T_{out}, x_{out}, P_{el}$	-	<p>performance maps of turbocompressor:</p> $\dot{m} = f(N_c, \beta), \eta_p = f(N_c, \beta)$
Gas storage	Dy	$\dot{m}_{in}, T_{in}, x_{in}$	$p_{stor}, T_{stor}, x_{stor}$	$p_{stor}, T_{stor}, x_{stor}$	$\frac{dm_g}{dt} = \dot{m}_{g,in} - \dot{m}_{g,out}$ $\frac{dT_g}{dt} = \frac{\Delta \dot{H}_g - c_v T_g \frac{dm_g}{dt} - m_g T_g \sum_i \frac{\partial c_v}{\partial w_i} \frac{dw_i}{dt}}{c_v m_g + m_g T_g \frac{\partial c_v}{\partial T}}$ $\Delta \dot{H}_g = \dot{H}_{g,in} - \dot{H}_{g,out} = [(\dot{m}_g c_p T)_{in} - (\dot{m}_g c_p T)_{out}]$ $p_i = \frac{m_i RT}{M_i V}$

Component	Al/Dy	Inputs	Outputs	States	Main governing equations
Water condenser	Dy	$\dot{m}_{in}, T_{in}, x_{in}$	$p_{node}, T_{node}, x_{node}$	$p_{node}, T_{node}, x_{node}$	$\frac{dm_g}{dt} = \dot{m}_{g,in} - \dot{m}_{g,out} - \dot{m}_{H_2O,cond}$ $\frac{dm_{h_2O}}{dt} = \dot{m}_{H_2O,cond} - \dot{m}_{H_2O,out}$ $\frac{dT_g}{dt} = \frac{\Delta \dot{H}_g - \dot{H}_{H_2O} - P - \dot{Q}_{sc} - c_v T_g \frac{dm_g}{dt} - m_g T_g \sum_i \frac{\partial c_v}{\partial w_i} \frac{dw_i}{dt}}{c_v m_g + m_g T_g \frac{\partial c_v}{\partial T}}$ $P = p \frac{dV_g}{dt}$ $\Delta \dot{H}_g = \dot{H}_{g,in} - \dot{H}_{g,out} = \dot{m}_g [(c_p T)_{in} - (c_p T)_{out}] + \dot{m}_{cond} r_v + [(\dot{m}_w c_p T)_{in} - (\dot{m}_w c_p T)_{out}]$ $\log_{10} p_s = A - \frac{B}{T+C}$ $\frac{dp_i}{dt} = \frac{RT}{M_i V} \sum_i \dot{m}_i - \frac{p_i}{V} \frac{dV}{dt} + \frac{p_i}{T} \frac{dT}{dt}$
Gas pipeline	Dy	$p_{in}, T_{in}, x_{in}, p_{out}$	$\dot{m}_{out}, T_{out}, x_{out}$	T_{pipe}	$\dot{m} = \text{sign}(\Delta p) \sqrt{\frac{ \Delta p \rho A c_s}{\frac{\lambda L}{D_{in}} + Z}}$ $\frac{dT_{out}}{dt} = \frac{1}{\rho c_v V} \left(\dot{m} [(c_p T)_{in} - (c_p T)_{out}] - \dot{Q}_w \right)$
Heat pump	Al	T_h, T_c, P_{el}	P_{thout}, P_{thin}	-	$COP = \frac{COP_{nom}}{C_c(1-(1-C_c))} \frac{P_{el,nom}}{P_{el}}$
Gas pressure reduction valve	Al	p_{in}, T_{in}, x_{in} $p_{out}, T_{out}, x_{out}$ ϕ	$\dot{m}_{out}, T_{out}, x_{out}$	-	$Y = 1 - \frac{1}{3} \left(\frac{x}{F_k x_T} \right)$ $\dot{m} = N_x c_v Y \sqrt{x p_{in} \rho_{in}} \quad \text{if } \frac{2}{3} \leq Y \leq 1$ $\dot{m} = N_x c_v Y \sqrt{x_T p_{in} \rho_{in}} \quad \text{if } Y = \frac{2}{3}$
Boiler	Al	\dot{m}_f	P_{th}	-	$\dot{Q} = \eta_{eff} (\dot{m}_f LHV)$ $\eta_{eff} = \frac{\Lambda - \Lambda_{min}}{1 - \Lambda_{min}} (\eta_{nom} - \eta_{min}) + \eta_{min}$
Pump	Al	n, H	\dot{m}_w	-	<p>Characteristic curve based on the parameters:</p> $\pi_1 = \frac{gH}{n^2 D^2} \quad \text{and} \quad \pi_2 = \frac{\dot{V}}{n D^3}$ $p_w = p_a = p_{a,0} \left(\frac{V_{a,0}}{V_{a,0} - (V_w - V_{w,0})} \right)^k$
Expansion vessel	Dy	$\dot{m}_{in}, \dot{m}_{out}$	p_w	V_w	

Component	Al/Dy	Inputs	Outputs	States	Main governing equations
Water pipeline	Dy	$\dot{m}_{w,in}$, p_{out}	$T_{w,in}$, $\dot{m}_{w,out}$, $T_{w,out}$	$T_{w,pipe}$	$Mc_w(T_{w,in}) \frac{dT_w}{dt} = \dot{m}c_w(T_{w,in})(T_{w,in} - T_w) - AU(T_w - T_{ext})$ $\Delta p = \Delta p_{geo} + \Delta p_{dist} + \Delta p_{conc}$ $\Delta p_{geo} = \rho_w g(z_{in} - z_{out})$ $\Delta p_{dist} = \lambda \rho_w \left(\frac{L}{\phi_{in}} \frac{v^2}{2} \right)$ $\Delta p_{conc} = \rho_w \frac{v^2}{2} k_r$ $\frac{1}{\rho_w A_{in}} \frac{d\dot{m}}{dt} = \frac{(p_{max} - p_{min} - \sum_i (\Delta p)_i) A_{in}}{\sum_i M_i}$
Heat changer	ex-Dy	$\dot{m}_{w,in}$, $p_{w,in}$, P_{th}	$T_{w,in}$, $p_{w,out}$, $T_{w,out}$	T_w	$\Delta p_{conc} = \rho_w \frac{v^2}{2} k_r,$ $Mc_w(T_{w,in}) \frac{dT_w}{dt} = \dot{m}c_w(T_{w,in})(T_{w,in} - T_w) + \dot{Q}$

Table 1: System components summary. (Al = Algebraic, Dy = Dynamic, H = pressure head, n = pump rotational speed, w = water, f = fuel, ϕ = valve opening)

3 Digital twin of the case study

3.1 Model of the case study

The case study considered consists of a PtG plant for the production of synthetic methane, using the renewable electricity generated by a wind power plant. A simplified representation of the energy system is displayed in Figure 5, while the layout of the digital twin developed in Simulink® is shown in Figure 6.

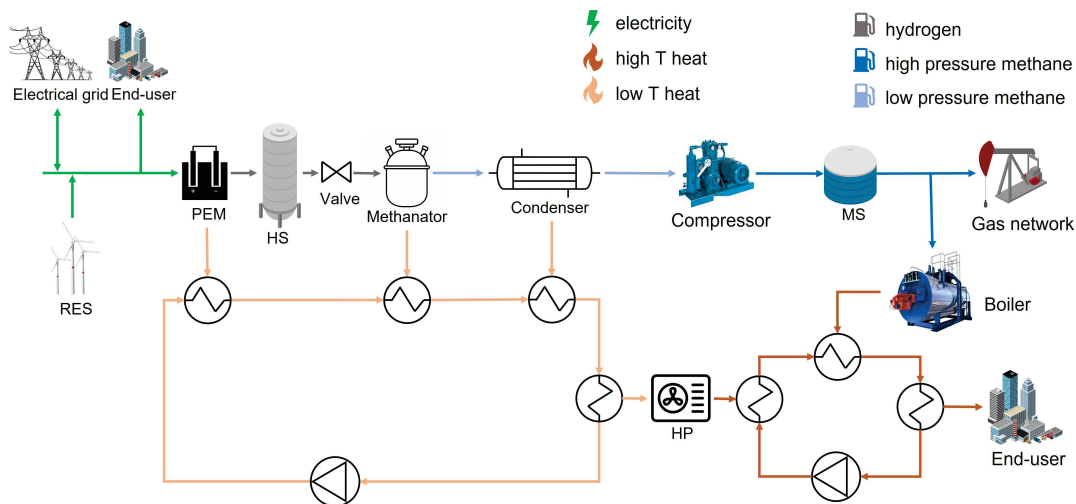


Figure 5: Schematization of the Multi-Energy System considered. (HS = hydrogen storage, MS = methane storage)

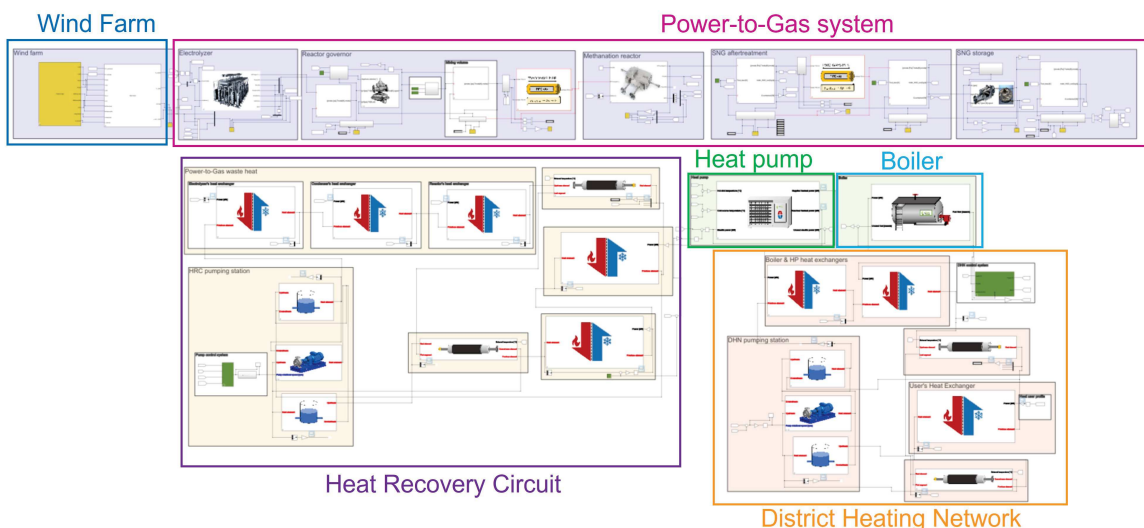


Figure 6: Digital twin of the PtG plant with waste heat recovery and use in a DHN.

The energy system is connected to the electrical grid and to the natural gas network, and it can exchange electricity and gas with them by buying and selling energy. The end-user has both electrical and thermal needs: the first are fulfilled by using the

renewable electricity or by buying electricity from the power grid, while the latter are met with a gas-fueled boiler, and by recovering the waste heat from the PtG plant. Indeed, as aforementioned, two hot water circuits are used: the HRC that works at low temperature ($40\div 55$) °C, in which three heat exchangers recover the waste heat from electrolyzer (available at a temperature of 55 °C), condenser (80 °C) and methanation reactor (290 °C), and the DHN which works at higher temperatures ($60\div 80$) °C and it is used for end-user heat supply (see Figure 5). An industrial heat pump (HP) connects the two circuits and upgrades the heat at 55 °C to the 80 °C needed for the DHN. The characteristics of the plants are exposed in Table 2.

In Figure 7, all the energy flows involved are shown: the electricity produced by the wind farm can be used both for the fulfillment of the electrical needs, or by the PEM electrolyzer (PEM) that produces hydrogen, and it is also consumed by the methane compressor and by the HP. The produced hydrogen can be stored in the hydrogen storage (HS) or used by the methanation reactor, which produces methane at low pressure (2.5 bar), that needs to be compressed before being stored in the methane storage (MS) or used. After the compression, the methane can both be stored, sold to the grid, or used to feed the boiler, which produces the heat for end-user supply.

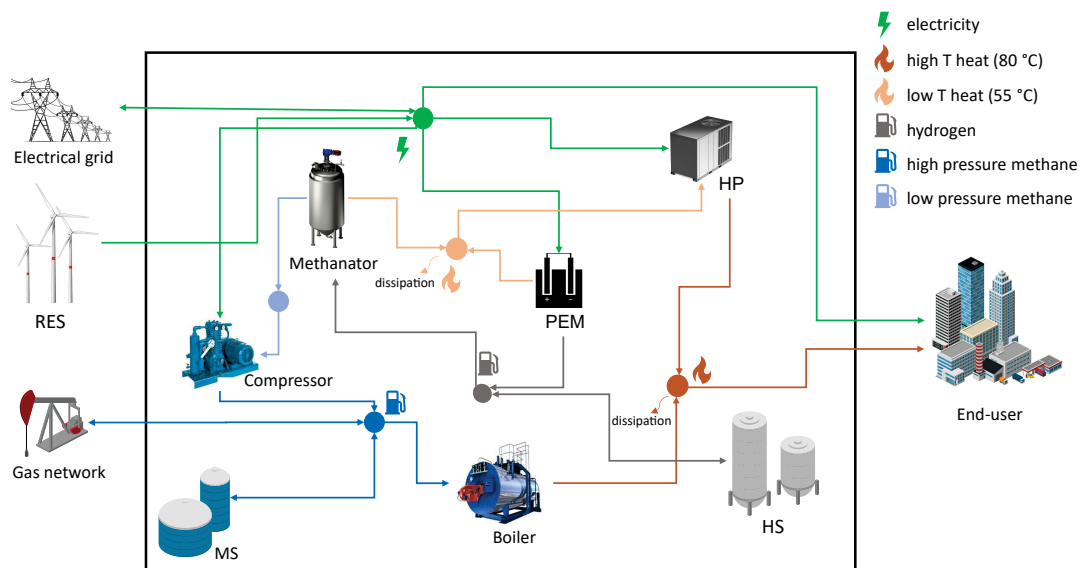


Figure 7: Energy flows involved in the Multi-Energy System considered. (HS = hydrogen storage, MS = methane storage)

The system can be simulated for the desired time interval. The main goal of the system is to fulfill these requirements:

- The electrical load of the end-user must be fulfilled, either by using the renewable electricity produced by the wind farm, or by buying it from the power grid.
- Similarly, the thermal load of the end-user is fulfilled through the DHN, which uses the heat produced by the boiler or by the heat pump, that extracts the heat from the HRC.

Table 2: Characteristics of the plants involved.

Technology	Parameter	Value
Wind farm	Number of turbines (-)	4
	Nominal power (kW)	8000
Electrolyzer	Nominal inlet power (kW)	3750
	Nominal operating temperature (°C)	55
	Nominal operating pressure (bar)	35
Methanator	Nominal inlet power (kW)	2479
	Nominal operating temperature (°C)	290
	Nominal operating pressure (bar)	2.5
Boiler	Nominal inlet power (kW)	4000
	Nominal efficiency (%)	92.4
Heat pump	Nominal inlet power (kW)	380
H ₂ storage	Volume (m ³)	100
	Maximum pressure (bar)	35
	Minimum pressure (bar)	2.5
Methane storage	Volume (m ³)	100
	Maximum pressure (bar)	7.5
	Minimum pressure (bar)	3.5

- All the electricity produced by the wind farm needs to be allocated, either using the PtG system or by selling it to the power grid.

3.2 System control

The system can be simulated for the desired time interval, as long as the evolution over time of the wind power production, heating and electrical load is provided. For the management of the system, a suitable and efficient rule-based control was developed, that permits to calculate the set-points which are given to low-level controllers. The set-points are calculated based on the logic displayed in Table 3.

It needs to be mentioned that the boiler set-point is not calculated with this control logic, and its input power is regulated through a PI controller, which keeps the supply temperature of the DHN equal to 80 °C. In addition, the actual amount of methane exchanged with the network is the difference between the set-point given for the methane sold and the methane needed for the boiler.

3.3 Simulation results

The system can be simulated for the desired time span, and the results can be collected and analyzed. In this section, the results obtained with a one-day simulation are exposed. The disturbances given to the digital twin are the electricity and thermal needs of the end-user, and the wind power produced by the wind farm, and they are shown in Figure 8.

Table 3: Rule-based control strategy definition.

Variable	Condition	Set-point value
Electrolyzer SP	$SoC_{HS} \leq 80\%$ otherwise	$\min \{P_{nom}, (P_{wind} - P_{el_{user}})\}$ 0
Methanator SP	$SoC_{HS} > 60\% \ \& \ SoC_{MS} \leq 95\%$ $SoC_{HS} > 60\% \ \& \ SoC_{MS} > 95\%$ otherwise	P_{nom} $0.5 P_{nom}$ 0
Heat pump SP	methanator ON & $P_{th_{user}} > 0$ otherwise	P_{nom} 0
Boiler SP	—	—
Methane sold	$SoC_{MS} > 70\%$ $30\% \leq SoC_{MS} \leq 70\%$ $SoC_{MS} < 30\%$	1200 kW 600 kW 0 kW

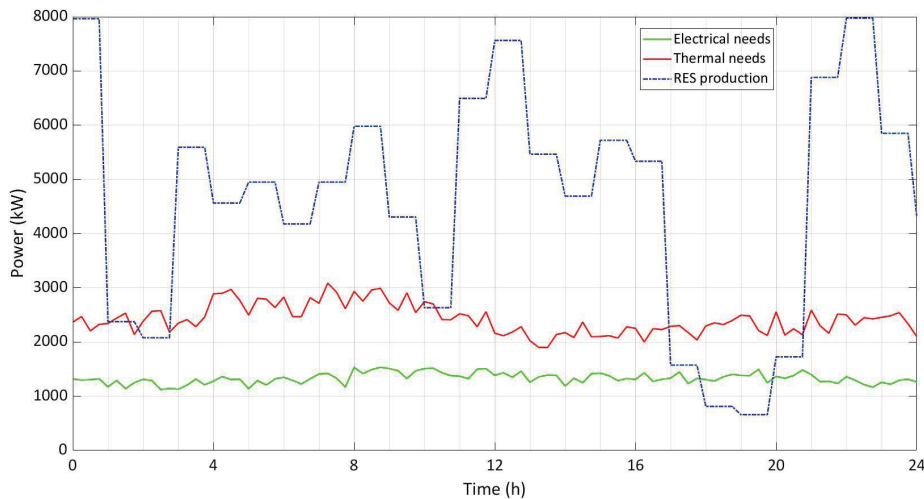


Figure 8: Disturbances given to the model over the simulated day.

During the simulated day, the electricity is allocated as shown in Figure 9: besides fulfilling the user electrical needs, the rest of the electricity is used to work the electrolyzer and generate hydrogen and then methane, and the remaining is sold to the grid. It can be noted that the electrolyzer is switched off in some moments, even though the wind farm production is not null: this happens when the hydrogen storage is full, as it is displayed in Figure 10. Here, both hydrogen and methane storage State of Charge (SoC) are shown. Finally, Figure 11 shows the methanation reactor management: both the set-point and the actual behavior of the methanator are shown. The set-point takes into consideration the set-point from the rule-based control and a correction based on the behavior of the hydrogen storage that avoid the storage to exceed its limits. It is shown that the actual management is able to follow the set-point quite precisely.

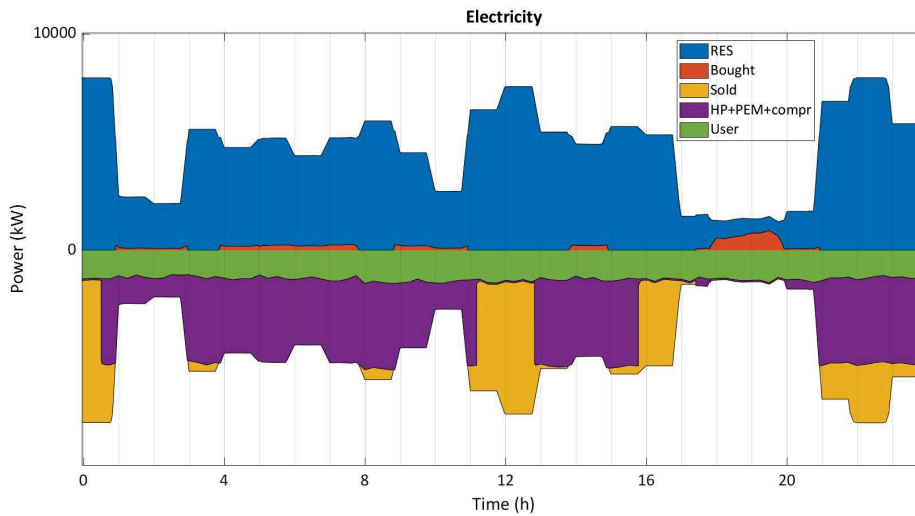


Figure 9: Electricity management over the simulated day.

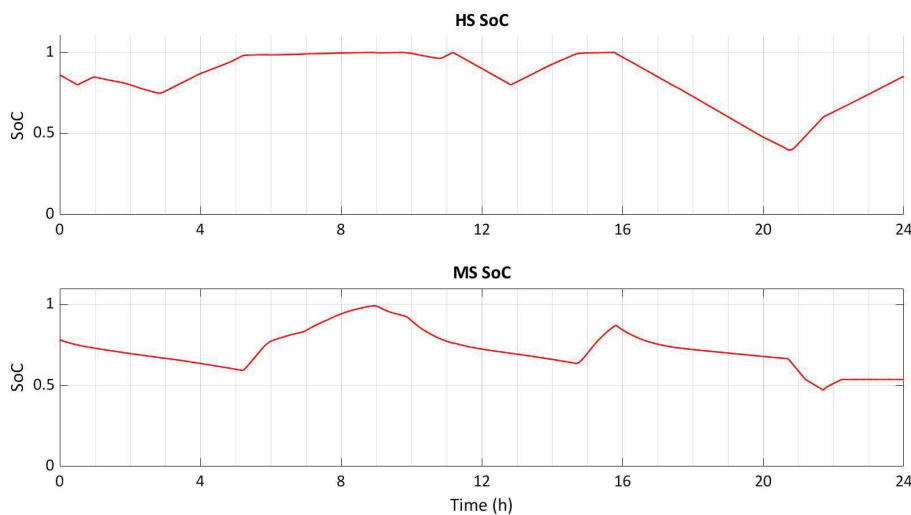


Figure 10: Hydrogen and methane storage management over the simulated day.

4 Conclusions

In this report, the activities of the second task of WP3 are reported. The detailed dynamic model of a Power-to-Gas system coupled with a district heating network for heat recovery was built in the MATLAB®/Simulink® simulation environment. A library of energy system components developed by the research group of the University of Parma was used. Firstly, the main sub-models representing the energy conversion units and storage systems (wind farm, electrolyzer, methanator reactor, water condenser, gas compressor, gas storage, gas pipeline and heat pump) were described. The components of the district heating network were summarized. Then, the way in which these modular components were assembled to form the digital twin of the case study was illustrated. Finally, the control logic implemented to achieve the desired operation is

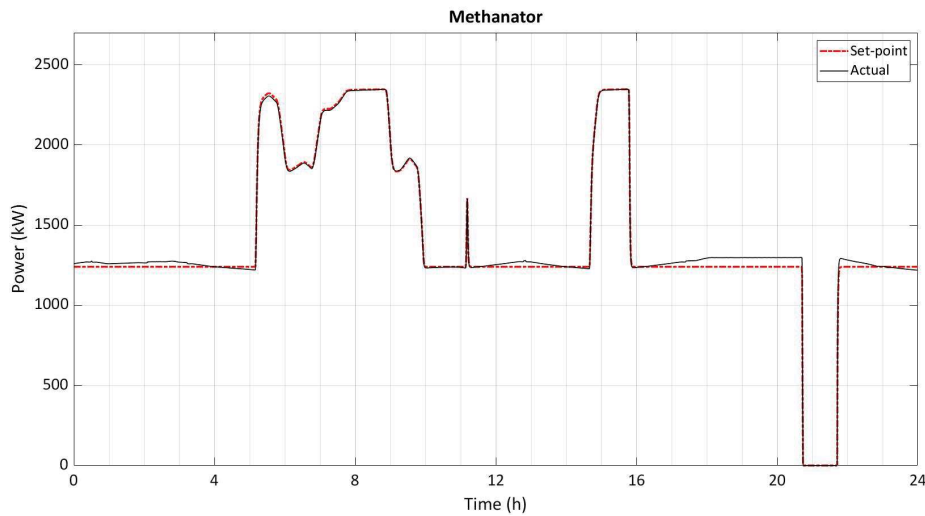


Figure 11: Methanation reactor management over the simulated day.

summarized and a preliminary analysis of the computational feasibility of the simulator was carried out.

The output of the task is a complete simulation platform representing the energy system of a Power-to-Gas system coupled with a district heating network for heat recovery. The model will be used to test the new control strategy based on Model Predictive Control developed in T3.3 and to compare it with a conventional control approach.

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