

THE ROLE OF METHANATION MODELING IN THE SIMULATION OF POWER-TO-GAS SYSTEMS

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ABSTRACT

The role that green hydrogen can play in the future energy systems has been undergoing huge investigations in recent years due to its versatility of use and its exiguous greenhouse impact. However, this energy carrier exhibits low volumetric energy density, difficulties in transportation, and high storage costs. Therefore, if not used at the site of production, it needs to be converted into other carriers for transportation and use. In this framework, synthetic methane can represent a valid option if used as a natural gas substitute taking advantage of its transportation infrastructures. Renewable methane can be synthesized from green hydrogen and captured carbon dioxide in power-to-gas systems.

In order to optimize the efficiency of methane production, these systems need to be integrated into larger energy networks where it is possible to benefit from the exploitation of energy in its variety of forms (e.g. electrical, thermal, and chemical). For this reason, the employment of mathematical models is essential for optimal process development. Depending on the purpose of a specific simulation and the time horizon, it is necessary to approach the study with the most suitable level of modeling detail.

In this work, the methanation technology is analyzed in the context of power-to-gas on multiple level modeling. Indeed, in several cases, methanation modeling requires the capability to capture characteristics of the input hydrogen such as mass flow rate, moisture content, or pressure. However, in other cases, the focus can regard the whole system operation and control. In such circumstances, the need to analyze specific component characteristics leaves room for considerations of mass and energy transfers, and component operating conditions and efficiencies.

The paper at hand proposes and combines two modeling approaches. The choice of a specific approach is suggested considering the obtainment of all the information to be gathered from a specific simulation. The results of the interaction of the methanation reactor with other power-to-gas components are provided.

1 INTRODUCTION

The power-to-gas process is based on the conversion of electrical energy into chemical energy in the form of a gaseous fuel allowing long-term energy storage. The process steps include the production of green hydrogen through renewable-powered electrolysis, and the conversion into methane through its reaction with carbon dioxide. If the carbon dioxide used were previously captured, this process would be free from climate-altering emissions. According to the stoichiometry of the methanation reaction, one mole of carbon dioxide and four moles of hydrogen are required to obtain one mole of methane and two moles of water.

By coupling electrolyzers and methanation reactors, such processes are complex and have not yet been thoroughly researched (Barbaresi *et al.*, 2022). For these reasons, the use of mathematical models can be greatly beneficial in increasing their technology readiness level quickly and economically. In general, simulations can help in component sizing, in system layout design, and in defining control strategies. Models are needed that describe individual components as well as models that consider the entire system.

In this field, few studies have employed multiple modeling approaches. Regarding component insights, Fischer *et al.* (2019) investigated wall-cooled fixed-bed reactors for carbon dioxide methanation with models ranging from homogeneous one-dimensional to heterogeneous two-dimensional. With increasing detail, models were able to better capture the reaction dynamics. Comparing homogeneous and heterogeneous reactor models, Schlereth and Hinrichsen (2014) went into further detail considering a pellet-level spatial scale for the catalyst bed. Modeling the intraparticle mass transport was found to be fundamental in examining the heat transfer limitations occurring in reactors with a small pore diameter and operated with small Reynolds numbers. Fambri *et al.* (2022) analyzed the problem on a system level considering the power-to-gas in distribution networks. Electricity grid models that are too approximated were indicated to be ineffective in the calculation of the ability of power-to-gas plants to absorb surplus renewable energy with non-negligible under- or over-estimations.

Nevertheless, none of the existing studies investigated the role that methanation modeling can play in power-to-gas systems analyses. This paper aims to fill this gap by presenting multiple methanation modeling approaches with different levels of detail. As a demonstration of the model capabilities, each approach was applied to the case studies for which the chosen model is considered the most appropriate. Specifically, in section 2 a mathematical model suitable for component analysis will be proposed. Considerations will be given about the role of the methanation reactor when coupled with electrolyzers. Section 3 will regard a simpler model of a methanation unit included in the entire power-to-gas system. Simulation results on the system behavior over longer timespans will be presented. In section 4, some remarks on models for optimization and control will be provided. Lastly, conclusions will be drawn in section 5.

2 COMPONENT INSIGHTS

Depending on the purposes, models of methanation reactors can range from simple algebraic (Koytsoumpa and Karellas, 2018) to particularly complex (Gruber *et al.*, 2021). They can be utilized to calculate the reaction progression along the reactor as well as the temperature profile. If the dynamics is envisaged, they can be used to simulate the reactor operation in particular transient conditions. Catalyst activity and thermal aspects can also be investigated. Furthermore, these kinds of models can be used to maximize the efficiency and to design the reactor.

Nonetheless, too complex models can overload the computational time as they consider aspects that may not be relevant to the case under investigation. Moreover, the use of a large number of parameters can lead to misleading results since each parameter brings a certain approximation. In addition, model parameters are often tuned only within specific operating ranges.

The advantages and disadvantages of component models are summarized by means of a strength, weaknesses, opportunities, and threats (SWOT) analysis in Table 1.

2.1 Mathematical model

In this work, a one-dimensional dynamic mathematical model was chosen for the component analysis. It regarded an heterogeneous tubular fixed-bed chemical reactor suitable for methanation purposes. Mass and energy balances as well as chemical kinetics are the fundamental equations on which the model was based.

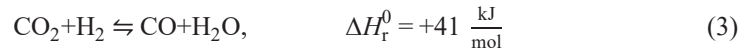
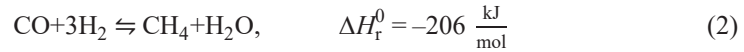
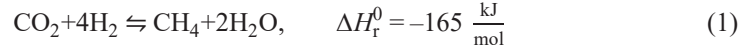
The model was spatially discretized. The reactor was divided into ten control volumes arranged in series along the reactor axis. A lumped parameter approach was employed. Therefore, in each control volume, gas properties were considered homogeneous.

Table 1: Component model SWOT analysis.

Strengths	Weaknesses	Opportunities	Threats
Fidelity to the real physical behavior	High computational costs	Decoupling of effects that are physically correlated	Risk of errors caused by parameters tuning approximation

The flow was considered one-dimensional as its signal passed from one control volume to the next. Each control volume exchanged heat radially with respect to the outside environment. The equations of the model were implemented in a MATLAB®/Simulink® environment and solved by the variable time step solver ode15s.

The three main reactions taking place in the methanation process were considered (Götz *et al.*, 2016). Specifically: carbon dioxide methanation (cdm, Eq. (1)), carbon monoxide methanation (cmm, Eq. (2)), and reverse water gas shift (rwgs, Eq. (3)).



The reaction kinetics was accounted for with the correlations for the reaction rates proposed by Xu and Froment (1979):

$$r_{\text{cdm}} = \frac{\frac{k}{p_{\text{H}_2}^{3.5}} \left(p_{\text{CH}_4} p_{\text{H}_2}^2 \text{O} - \frac{p_{\text{H}_2}^4 p_{\text{CO}_2}}{K} \right)}{\left(1 + B_{\text{CO}} p_{\text{CO}} + B_{\text{H}_2} p_{\text{H}_2} + B_{\text{CH}_4} p_{\text{CH}_4} + \frac{B_{\text{H}_2\text{O}} p_{\text{H}_2\text{O}}}{p_{\text{H}_2}} \right)^2} \quad (4)$$

$$r_{\text{cmm}} = \frac{\frac{k}{p_{\text{H}_2}^{2.5}} \left(p_{\text{CH}_4} p_{\text{H}_2} \text{O} - \frac{p_{\text{H}_2}^3 p_{\text{CO}}}{K} \right)}{\left(1 + B_{\text{CO}} p_{\text{CO}} + B_{\text{H}_2} p_{\text{H}_2} + B_{\text{CH}_4} p_{\text{CH}_4} + \frac{B_{\text{H}_2\text{O}} p_{\text{H}_2\text{O}}}{p_{\text{H}_2}} \right)^2} \quad (5)$$

$$r_{\text{rwgs}} = \frac{\frac{k}{p_{\text{H}_2}} \left(p_{\text{CO}} p_{\text{H}_2} \text{O} - \frac{p_{\text{H}_2} p_{\text{CO}_2}}{K} \right)}{\left(1 + B_{\text{CO}} p_{\text{CO}} + B_{\text{H}_2} p_{\text{H}_2} + B_{\text{CH}_4} p_{\text{CH}_4} + \frac{B_{\text{H}_2\text{O}} p_{\text{H}_2\text{O}}}{p_{\text{H}_2}} \right)^2} \quad (6)$$

Arrhenius-type temperature functions were used for the calculation of reaction rate coefficients k , reaction equilibrium constants K , and adsorption constants B .

The mass balance equation (Eq. (7)) considers the flows of the chemical species entering and exiting the control volumes as well as the formation of products and the disappearance of reactants.

$$\varepsilon S V \frac{\partial \rho_a}{\partial t} = (Q_{v,\text{in}} \rho_{a,\text{in}} - Q_v \rho_a) + \dot{m}_{a,\text{gen}} \quad (7)$$

Volumetric flow rate Q_v was calculated accounting for bed porosity ε as follows:

$$\dot{m}_a = \rho_a Q_v = \rho_a \varepsilon S u \quad (8)$$

$$\varepsilon = V_{\text{void}} / V_{\text{tot}} \quad (9)$$

The flow speed u calculation was based on the calculation of the pressure drops which were evaluated with the Ergun equation (Ergun and Orning, 1949).

$$u = \sqrt{\left(\frac{\Delta p \psi d_p}{f l \rho} \right)} \quad (10)$$

with:

$$f = \frac{1-\varepsilon}{\varepsilon^3} \left(1.75 + 150 \frac{1-\varepsilon}{\psi d_p \rho u / \mu} \right) \quad (11)$$

The source term $\dot{m}_{\alpha, \text{gen}}$ denotes the mass flow rate generated (or removed if negative) by means of the chemical reactions. It was calculated according to the following Equation (12).

$$\dot{m}_{\alpha, \text{gen}} = S \rho_{\text{cat}} (1 - \varepsilon) M_{\alpha} \sum_j v_{\alpha j} r_j \quad (12)$$

The energy balance (Eq. (13)) considered the enthalpy of the gases entering and exiting the control volumes, as well as the thermal power generated by the exothermal reactions, and the thermal power exchanged radially toward the outside environment.

$$S K C_{\text{eff}} \frac{\partial T}{\partial t} = \sum_{\alpha} (\dot{m}_{\alpha, \text{in}} h_{\alpha, \text{in}} - \dot{m}_{\alpha} h_{\alpha}) + \dot{Q}_{\text{gen}} - \dot{Q}_{\text{r}} \quad (13)$$

The effective thermal capacity C_{eff} was calculated with Equation (14).

$$C_{\text{eff}} = (\rho c)_{\text{eff}} = \rho_{\text{cat}} c_{\text{cat}} (1 - \varepsilon) + \varepsilon \sum_j \rho_j c_{v, j} \quad (14)$$

Source and sink terms in Equation (13) were calculated as follows:

$$\dot{Q}_{\text{gen}} = S \rho_{\text{cat}} (1 - \varepsilon) \sum_j \Delta H_j r_j \quad (15)$$

$$\dot{Q}_{\text{r}} = U A \Delta T \quad (16)$$

where the global heat transfer coefficient U was considered constant.

2.2 Application results

A detailed model of the methanation reactor allows the investigation of specific aspects of the component. Here, the reactor conversion trends in conditions relevant for power-to-gas applications are considered. The conversion ζ was calculated for both reactants, i.e. hydrogen and carbon dioxide, with the following equation:

$$\zeta = \frac{\dot{n}_{i, \text{in}} - \dot{n}_{i, \text{out}}}{\dot{n}_{i, \text{in}}} \quad (17)$$

where the inlet and outlet mole flow rates of a generic reactant are considered.

Considering the coupling with renewable-powered electrolysis, it is interesting to evaluate the behavior of the methanation reactor by varying the flow rate of the reactants. In fact, the hydrogen production is proportional to the intermittent electrical energy input in the electrolyzer. Following the hydrogen production, the modulation of the methanation unit inlet flow rate may also be necessary.

Figure 1 shows hydrogen and carbon dioxide conversion with increasing gas hourly space velocity $GHSV$, a parameter indicating the volumetric inlet flow rate per unit reactor volume. For values of $GHSV$ higher than approximately 6000 h^{-1} , the reactant conversion underwent a sharp decrease due to lower residence times. The decrease resulted in a higher concentration of unconverted reactants in the outlet gas mixture. This affected its purity and usability.

As the $GHSV$ increased, the peak temperature that was reached in the reactor increased due to greater energy release from the exothermal reactions involved (see Eqs. (1)–(3)). The increase in temperature has a negative effect on the chemical equilibrium of exothermic reactions, resulting in reduced conversion. It is also noticeable that the trend for hydrogen conversion differed from that for carbon dioxide. At $GHSV$ s higher than 5000 h^{-1} , in fact, the two curves began to diverge.

This behavior can be explained by considering that at high temperatures the endothermic reverse water gas shift reaction (Eq. (3)) is favored, which resulted in the formation of small amounts of carbon monoxide.

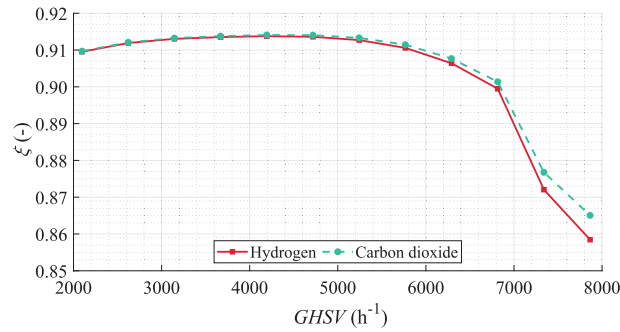


Figure 1: Hydrogen and carbon dioxide conversion with increasing gas hourly space velocity.

In such cases, the carbonaceous constituent of carbon dioxide was not converted exclusively into methane but also, to a smaller extent, into carbon monoxide. These results agree with the *GHSV* ranges commonly used in practice (Götz *et al.*, 2014).

When dealing with power-to-gas systems with direct coupling between water electrolysis and methanation, it is important to evaluate the effects that the presence of water vapor could have on methanation. Figure 2 (a) shows the consequences on conversion that an inlet humid flow of hydrogen has on the conversion of the two reactants. This referred to a condition in which the moisture content was present only in the hydrogen flow, while the carbon dioxide flow rate was constant and equal to the stoichiometric value it would have with dry hydrogen.

For comparison, the simulation shown in Figure 2 (b) isolated the effect that water has on methanation. The figure depicts the variation of the moisture content in the mixture entering the reactor, in each case maintaining the stoichiometric ratio between carbon dioxide and hydrogen. For the sake of clarity, the mole fractions of the inlet gases in the two cases are given in Table 2.

It can be seen from Figure 2 (a) that the increase in inlet moisture content led to a modest improvement in hydrogen conversion. In that case, the hydrogen in the reactant mixture assumed sub-stoichiometric values and the conversion was gradually more effective. Conversely, in such cases carbon dioxide was over-stoichiometric. For this reason, the conversion of carbon dioxide was greatly reduced as the amount of water increased. Therefore, although hydrogen can be converted effectively, the purity of synthetic methane is undermined by the presence of water at the inlet.

Additional information can be gained by analyzing Figure 2 (b). In this case, keeping the reactant ratio at the stoichiometric value, the model could isolate the effect that water has on the development of the methanation reaction. In this case, both the hydrogen and carbon dioxide conversion underwent a net decrease. This can be explained by considering that water is one of the two products of the methanation reaction. The presence of one of the products in the inlet mixture results in a shift in the chemical equilibrium that counteracts the formation of the products.

The effect of water highlighted by Figure 2 (b) contributes to the explanation of why the decrease in carbon dioxide conversion is so pronounced and why the hydrogen conversion curve has a local maximum with mole fractions of inlet water of around 0.45. In fact, in the second case, for larger quantities, the detrimental effect related to the equilibrium shift highlighted by Figure 2 (b) exceeds the increase in hydrogen conversion due to the over-stoichiometric carbon dioxide.

Table 2: Inlet mole fraction of the species in the analysis depicted in Figure 2.

X_{in}	Moisture in the hydrogen flow (Figure 2 (a))	Moisture in the stoichiometric reactant mixture flow (Figure 2 (b))
CO ₂	0.2	0.2 (1 - $X_{H_2O,in}$)
H ₂	0.8 - $X_{H_2O,in}$	0.8 (1 - $X_{H_2O,in}$)
H ₂ O	$X_{H_2O,in}$	$X_{H_2O,in}$

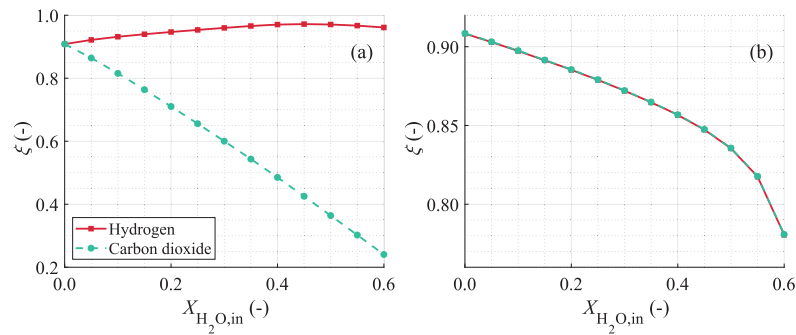


Figure 2: Hydrogen and carbon dioxide conversion with increasing inlet moisture content in the hydrogen flow (a), and in the gas mixture keeping the reactant stoichiometric ratio (b).

Figure 3 shows the effect of the system operating pressure on conversion. An increase in the operation pressure of the methanation reactor had a beneficial effect on both hydrogen and carbon dioxide conversion. This increase was most pronounced up to about 10 bar, while above this pressure, the conversion continued to improve but less significantly. This behavior is in agreement with the literature results (Kang and Lee, 2013).

Operation at relatively high pressures, therefore, contributes to increasing the system efficiency. In addition, in power-to-gas contexts where a storage unit is positioned before the methanation unit, the increase in hydrogen delivery pressure helps to reduce storage size and cost.

3 SYSTEM ANALYSIS

When system analysis is the main goal, model structures can vary notably. As an example, they can be based on the calculation of efficiencies (Salomone *et al.*, 2019) or of mass and energy flows (Kezibri and Bouallou, 2017).

Models designed for system analysis are often light enough to allow quick calculations. They can be utilized for long timespans (e.g. seasonal) analyses and for reproducing large networks. In fact, they can be integrated into larger contexts that may also include other models. Within the framework of power-to-gas, electrical models can be coupled with fluid dynamics and chemical models.

Besides the strengths, these models can also exhibit drawbacks. If the approximation is too high, the simulation results may deviate too much from the real physical behavior of the technology. Moreover, the validation of large system models can be difficult due to the number of sub-systems often not taken into consideration. The advantages and disadvantages are summarized by means of a SWOT analysis in Table 3.

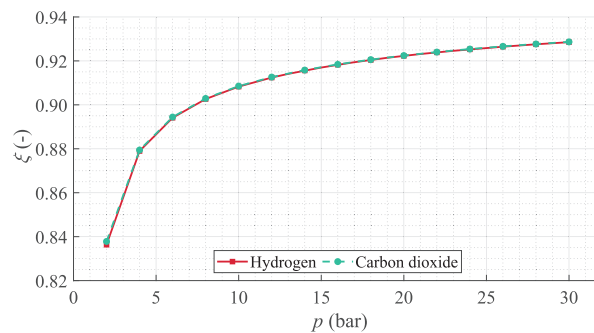


Figure 3: Hydrogen and carbon dioxide conversion with increasing pressure.

Table 3: System model SWOT analysis.

Strengths	Weaknesses	Opportunities	Threats
High speed calculations	Reduced physical accuracy	Possibility of coupling with other system models	Can be hard to validate with respect to real facilities

3.1 Mathematical model

In this work, a methanation reactor algebraic model was chosen for the system analysis. In contrast with the model presented in section 2, it accounted only for the reaction of carbon dioxide methanation. The methane yield y was calculated by means of a look-up table constructed by a linear fitting of experimental data from the literature (Bengaouer *et al.*, 2018), based on the gas hourly space velocity and reactant ratio.

$$y = a \left(\frac{GHSV}{GHSV_{nom}} \right) + b \quad (18)$$

Similar look-up tables can be constructed on the basis of more detailed models such as the one presented in section 2. The thermal power released by the exothermal reaction was expressed by the following equation:

$$\dot{Q}_{react} = y \dot{n}_{CO_2,in} \Delta H_r^0 \quad (19)$$

The thermal power needed to heat up the inlet gas to the temperature of the reactor was calculated with Equation (20).

$$\dot{Q}_{gas} = \dot{m}_{in} c_{p,mix} (T_{reactor} - T_{gas,in}) \quad (20)$$

The surplus thermal power was thus calculated as the difference between Equation (19) and Equation (20).

3.2 Application results

This model was applied for the investigation of the power-to-gas system represented in Figure 4. A renewable source (PV, located in Parma, Italy) was used to power an electrolyzer stack (nominal power equal to 3750 kW_e); the produced hydrogen was then directed into a storage tank. According to a rule-based control logic, a certain quantity of hydrogen was extracted from the storage tank and mixed with the corresponding stoichiometric quantity of carbon dioxide. The gas mixture was then conveyed to the methanation unit where the conversion into the products (methane and water) took place.

The methanation unit was operated at a pressure of 2.5 bar and a temperature of 290 °C. Downstream of this unit and after water condensation, the synthesized gas was dispatched into the natural gas distribution network. The control logic employed for the operation of the electrolyzer stack and the methanation unit followed the scheme depicted in Figure 5. It was applied at every simulation time step. This is only an example of possible control logic; no optimization was performed. The logic of the two components depended on the state of charge of the hydrogen storage tank, defined by the following Equation (21).

$$SoC_{H_2} = \frac{p - p_{min}}{p_{max} - p_{min}} \quad (21)$$

When the electrolyzer stack was ON, its power was set to be the minimum between the PV power and the electrolyzer nominal power. When the methanation unit was ON, the hydrogen and carbon dioxide quantities conveyed to the methanation reactor were proportional to the state of charge of the upstream hydrogen storage tank.

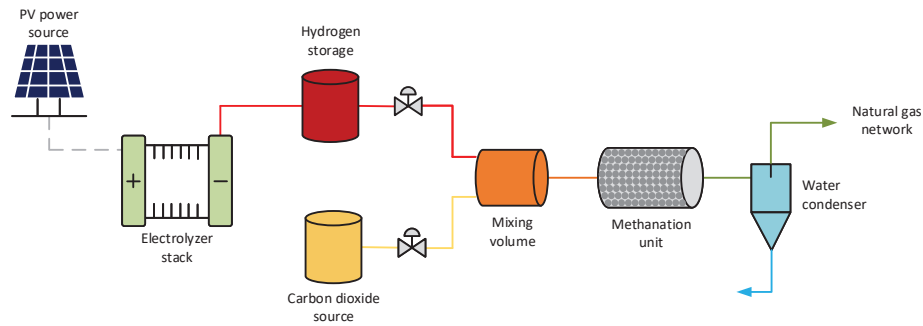


Figure 4: Modeled power-to-gas plant schematic diagram.

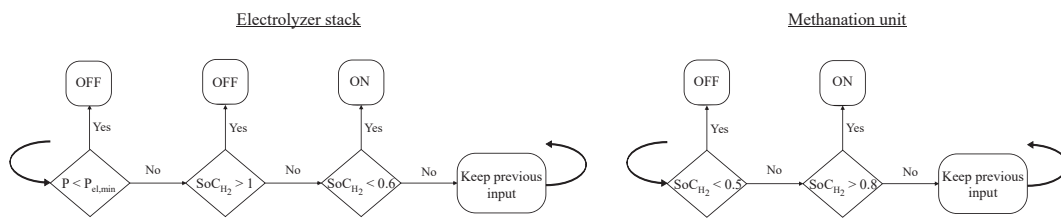


Figure 5: Control logic followed (and repeated at each time step) for the simulation of the power-to-gas system.

Figure 6 shows the effects of this control logic on the power-to-gas system for a week of operation. Specifically, in Figure 6 (a), the renewable power output is depicted; in Figure 6 (b), the operating mode (ON/OFF) of the electrolyzer stack and the methanation unit can be seen; and lastly, Figure 6 (c) shows the progress of the state of charge of the hydrogen storage placed between the electrolyzer stack and the methanation unit.

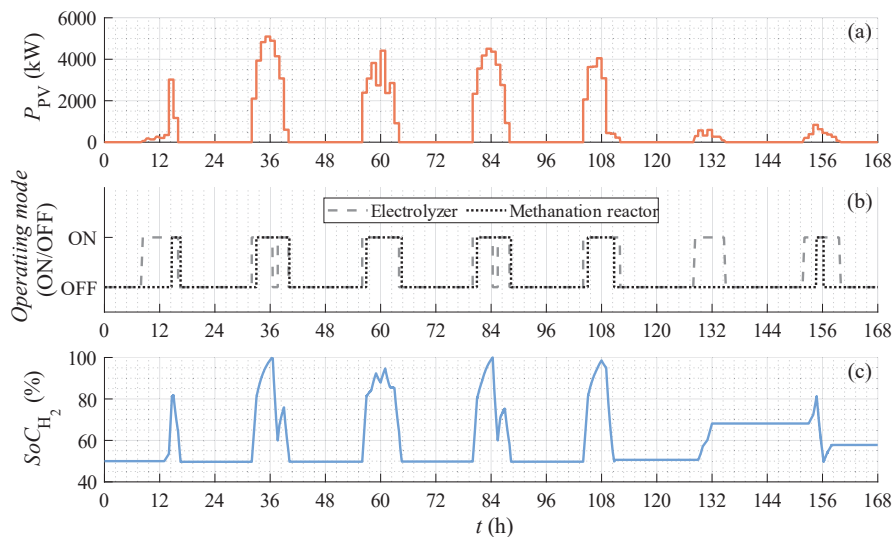


Figure 6: Simulated operation of the power-to-gas system. Photovoltaic power (a), electrolyzer and methanation reactor operating modes (b), hydrogen storage state of charge (c).

The switching ON of the electrolyzer stack and the methanation unit was affected by the trends of the upstream renewable energy source. Consequently, the state of charge of the hydrogen storage also exhibited significant variability. During the sixth day (visible at around hour 132), the methanation reactor was kept OFF due to the low availability of stored hydrogen.

Figure 7 focuses on the output of the methanation unit. The mass flow rate trends at the inlet of the methanation reactor are shown in Figure 7 (a); Figure 7 (b) shows the fuel power at the outlet (in terms of the lower heating value of the combustible species) together with the methane yield of the reaction; and lastly, Figure 7 (c) illustrates the mole flow rates of the chemical species at the outlet of the methanation reactor.

The inlet flow rate, noticeable in Figure 7 (a), was determined by the control logic presented previously. As can be seen from Equation (18), the methane yield (related to conversion efficiency) depends on the input flow rate. Indeed, in Figure 7 (b), the trend of methane yield, which inversely proportional to the flow rate, can be seen.

The chemical power available when there were high flow rates of reactants, plotted contextually with the yield, was proportional to the inlet mass flow rate but, due to the lower yield, exhibited larger amounts of unconverted hydrogen. Hydrogen, however, having low density, only slightly affected this aspect. In fact, from Figure 7 (c), it can be seen that the unconverted hydrogen had a greater weight in terms of mole flow rate.

4 SMART CONTROL AND OPTIMIZATION

When referring to multi-energy systems with integrated power-to-gas solutions, mathematical models capable of optimizing the system with a defined objective, such as cost or energy consumption minimization, are essential to enable smart system operation.

For instance, model-based optimization algorithms can be embedded in smart control approaches such as model predictive control. Using this control strategy, at every time step the controller calculates the optimal system operation over a prediction horizon by using an optimization algorithm with an integrated simplified model of the system to be controlled.

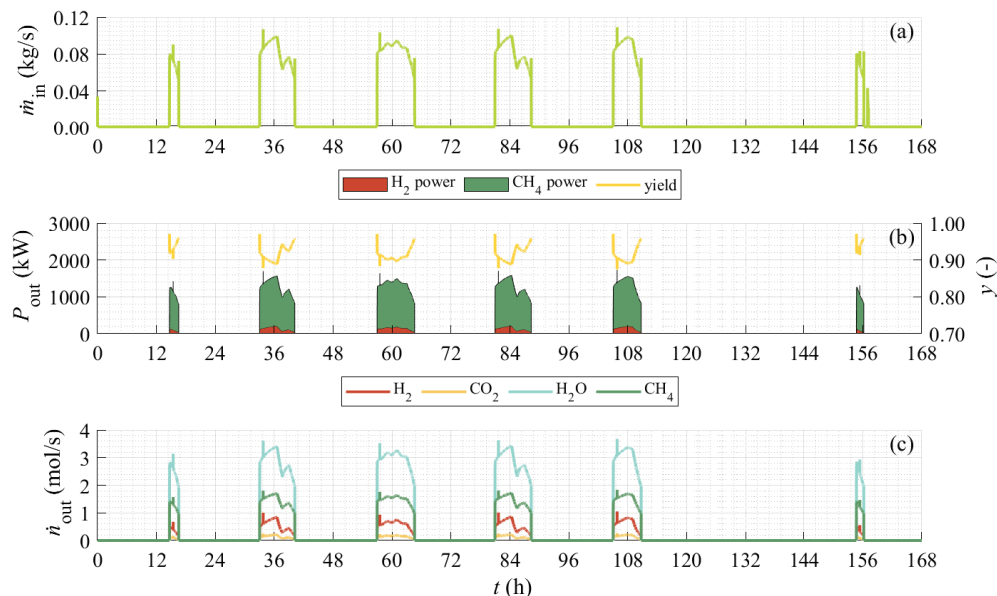


Figure 7: Simulated behavior of the methanation unit. Inlet reactant mass flow rate (a), produced fuel power and methane yield (b), outlet gas mole flow rates (c).

As the optimization procedure needs to be ran multiple times, the algorithm embedded in the controller should be fast enough to reach the optimal solution in real time. Examples of suitable algorithms for these applications include mixed-integer linear programming, which requires linear models, and dynamic programming, which requires discrete models.

Techniques of this kind have been successfully applied to power-to-gas systems through a mixed-integer linear programming algorithm in (Marzi *et al.*, 2024). The methanation reactor was modeled by means of linear input/output relations concerning the inlet power (based on the hydrogen lower heating value) and the outlet power (based on the methane lower heating value), i.e. the reaction yield (see Eq. 18) was considered constant.

Using these modeling methods, the methanation reactor can play an important role because, if it is properly controlled, it can avoid upstream renewable energy curtailment, maximize system conversion efficiency and, thus, minimize operating costs.

5 CONCLUSIONS

Power-to-gas processes are receiving particular attention from the research community because they allow renewable electricity to be stored in the form of chemical energy. Two main sub-processes are involved: electrolysis for the generation of green hydrogen, and methanation for the subsequent conversion of hydrogen and carbon dioxide into methane. In contrast to hydrogen, a gaseous energy carrier such as methane permits the use of existing natural gas infrastructures and technologies without concentration limitations. In this perspective, the use of mathematical models is essential to obtain a detailed analysis of the interaction between the various components.

In this paper, multiple approaches applied to the mathematical modeling of methanation in power-to-gas contexts were analyzed. In particular, two mathematical models were presented, and their capabilities were demonstrated in analyses of possible power-to-gas applications. On the one hand, a first approach focused on a relatively detailed model appropriate for the study of the single component (methanation reactor). On the other hand, a second approach concerned a less detailed model that allowed the possibility of system investigations.

With reference to methanation, considerations regarding the component alone or as part of a system assume equal relevance. This paper aims to guide the model choice by analyzing the conditions in which their greatest potential can be derived.

The potential of the component model was shown by analyzing the conversion of the methanation reactor under different conditions occurring in power-to-gas systems. This model showed that, for optimal conversion, it is important to size the methanation reactor in order to limit the gas hourly space velocities, to consider a condensation unit between the electrolyzer and the methanation reactor, and, if possible, to operate the system at relatively high pressures.

Simulations with the system model showed that such models can be highly useful for testing management strategies based on the renewable energy input, obtaining information related to system efficiency under various conditions as well as data regarding synthetic fuel production.

The use of methanation technologies in power-to-gas contexts can be optimized by employing model-based optimization algorithms embedded in smart control approaches.

NOMENCLATURE

A	area	(m ²)
a	linear fitting constant	
b	linear fitting constant	
B	mass diffusion coefficient	
c	specific heat	(J/kg·K)
C	thermal capacity	(J/K)
c_p	specific heat at constant pressure	(J/kg·K)
c_v	specific heat at constant volume	(J/kg·K)
d_p	particle equivalent diameter	(m)
f	friction factor	(-)

$GHSV$	gas hourly space velocity	(h^{-1})
h	specific enthalpy	(kJ/kg)
K	reaction equilibrium constant	(-)
k	reaction rate coefficient	($kmol/kg_{cat} \cdot h \cdot bar$)
l	control volume thickness	(m)
\dot{m}	mass flow rate	(kg/s)
M	molar mass	(g/mol)
\dot{n}	mole flow rate	(mol/s)
P	power	(W)
p	pressure	(bar)
PV	photovoltaic	
\dot{Q}	thermal power	(W)
Q_v	volumetric flow rate	(m^3/s)
r	reaction rate	($kmol/kg_{cat} \cdot h$)
S	cross section	(m^2)
SoC	state of charge	(%)
SWOT	strengths, weaknesses, opportunities, threats	
T	temperature	(K)
t	time	(s)
u	flow speed	(m/s)
U	global heat transfer coefficient	($W/m^2 \cdot K$)
y	yield	(-)
ΔH	reaction enthalpy	(J/mol)
ΔH_r^0	standard reaction enthalpy	(J/mol)
ε	bed porosity	(-)
μ	dynamic viscosity	(Pa·s)
ν	stoichiometric coefficient	
ζ	conversion	(-)
ρ	density	(kg/m^3)
ψ	form factor	(-)

Subscript

cat	catalyst bed
cdm	carbon dioxide methanation
cmm	carbon monoxide methanation
eff	effective
el	electrolyzer
gen	generated
i	reactant index
in	inlet
j	reaction index
max	maximum
min	minimum
mix	gas mixture
nom	nominal
out	outlet
r	radial
react	reaction
rwgs	reverse water gas shift
tot	total
void	void
α	gaseous species

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