



10th International Conference on Applied Energy (ICAE2018), 22-25 August 2018, Hong Kong, China

Techno-economic uncertainty quantification and robust design optimization of a directly coupled photovoltaic-electrolyzer system

Diederik Coppitters^{a,b*}, Ward De Paepe^c, Francesco Contino^{a,b}

^a*Vrije Universiteit Brussel (VUB), Thermo and Fluid dynamics (FLOW), Pleinlaan 2, 1050 Brussels, Belgium*

^b*Vrije Universiteit Brussel (VUB) and Université Libre de Bruxelles (ULB), Combustion and Robust Optimization Group (BURN), 1050 Brussels, Belgium*

^c*University of Mons (UMONS), Thermal Engineering and Combustion Unit, Place du parc 20, 7000 Mons, Belgium*

Abstract

To solve the problem of large time shifts between renewable energy supply and user demand, power-to-H₂ is a well-known option. In this framework, previous studies have shown that the direct coupling of a photovoltaic array with an electrolyzer stack is a viable solution. However, these studies assumed perfectly known operating parameters to optimize the setup. Moreover, they focused on maximizing hydrogen and minimizing the energy loss, while the cost was not addressed. We have performed an optimization including uncertainty quantification (i.e. surrogate-assisted robust design optimization) for several locations with the Levelized Cost Of Hydrogen (LCOH) as objective. This paper provides the least sensitive design to uncertainties and shows which parameters are most affecting the variability of the LCOH for that design. The robust design optimization illustrates that the mean and standard deviation of the LCOH are non-conflicting objectives for the robust designs of all considered locations. The optimal robust design is established at the considered location with the highest average yearly solar irradiance, achieving a mean LCOH of 6.6 €/kg and a standard deviation of 0.72 €/kg. The discount rate uncertainty is the main contributor to the LCOH variation. Therefore, installing a PV-electrolyzer system in locations with a high average yearly solar irradiation is favorable for both the LCOH mean and standard deviation, while de-risking the technology has the highest impact on further reducing the LCOH variation. Future works will focus on including accurate probability distributions and adding batteries to the system.

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Peer-review under responsibility of the scientific committee of ICAE2018 – The 10th International Conference on Applied Energy.

Keywords: Levelized cost of hydrogen, Photovoltaic-electrolyzer system, Robust design optimization, Uncertainty quantification.

* Corresponding author. Tel.: +32-2-6292816; fax: +32-2-6292865.

E-mail address: dcoppitt@vub.be

Nomenclature

Symbols

$a_{\text{H}_2\text{O}}$	water activity
G	Irradiance, W/m^2
I	current, A
m	mass, kg
N	number of electrolyzer units
r	discount rate
T	temperature, K
U	voltage, V

Acronyms

DDO	Deterministic Design Optimization
LCOH	Levelized Cost Of Hydrogen, €/kg
RDO	Robust Design Optimization
UQ	Uncertainty Quantification

Subscripts

elec	electrolyzer
lim	limiting

1. Introduction

PhotoVoltaic (PV) systems are the fastest growing renewable energy technology in the world (> 50 GW annually) [1,2]. Therefore, next to wind energy technologies, solar PV systems are considered the main technology for large-scale renewable energy harvesting [2]. However, with solar energy being an intermittent energy source, PV systems are in need of energy storage to comply with time-flexible energy demand. Batteries are not appropriate for large-scale energy storage, due to their high energy leakage (1%-5% per hour) and low energy density compared to chemical storage [3]. To overcome these drawbacks, interest is growing to use hydrogen as an energy carrier [3]. By using solar energy to generate hydrogen in a PV-electrolyzer system [4-6], a viable solution is provided to store excess solar energy. To ensure an optimal operating point of the PV-electrolyzer system in conventional designs, Maximum Power Point Tracking (MPPT) and DC-DC converters are used as an indirect coupling solution. However, direct coupling avoids the use of this expensive equipment, resulting in a reduction of both cost and complexity [4].

In a directly coupled PV-electrolyzer system, maximizing the hydrogen production and minimizing the excess power production are commonly selected objectives [4,6,7]. While the latter is only an alternative for cost optimization, the Levelized Cost Of Hydrogen (LCOH) gives an explicit indication of the economic performance of the system [8]. To achieve an optimal PV-electrolyzer design, multi-objective Deterministic Design Optimization (DDO) is frequently applied [9,10]. Common DDO techniques applied to a PV-electrolyzer system are Genetic Algorithm (GA), Particle Swarm Optimization (PSO) and Imperialist Competitive Algorithm (ICA) [7].

Previously mentioned DDO methods assume exact model parameters. However, in real-life applications, technical and economic parameters are often subject to uncertainties. To quantify the variation in the system objective due to uncertain inputs (i.e. Uncertainty Quantification (UQ)), non-intrusive Polynomial Chaos Expansion (PCE) is one of the most used techniques [11]. By using PCE to acquire accurate statistics, surrogate-assisted Robust Design Optimization (RDO) aims to provide a design that is least sensitive to input variations. RDO gained much attention in many fields, including structural dynamics, aerospace, automobile and telecommunications [12].

This paper covers the modelling of the directly coupled PV-electrolyzer system, followed by the DDO, RDO and UQ results. As case-to-case uncertainty is considered, this paper provides a robust solution for the system.

2. System modelling

In this section, the PV-electrolyzer model and the considered locations are introduced. Thereafter, the optimization and uncertainty quantification are described, which aim to achieve optimal operating conditions under uncertainties.

2.1. PhotoVoltaic (PV) system and electrolyzer stack

A single diode model without parallel resistance is considered to represent a PV cell [13]. To characterize the PV cell behavior, we used the model presented by González-Longatt [14], which is a simplification of the model of Gow and Manning [15]. For the electrolyzer, a Proton Exchange Membrane (PEM) electrolyzer is selected, by reason of its fast response time (< 1 s) and full operational flexibility [16]. The implemented PEM model is described in [4].

2.2. Climate data

To analyze the effect of various climates, we used hourly solar irradiance and temperature data for one year in Johannesburg, San Francisco and Bern [17]. These locations receive an average solar irradiance of 2302 kWh/m²/y, 1842 kWh/m²/y and 1243 kWh/m²/y respectively, with an average ambient temperature of 16°C, 14.2°C and 10.7°C.

2.3. Design optimization and Uncertainty Quantification (UQ)

To achieve the optimal system configuration, the electrolyzer cells in series N_s and parallel N_p [4], the water activity $a_{\text{H}_2\text{O}}$ [4] and electrolyzer operating temperature T_{elec} [16] are selected as design parameters:

$$1 \leq N_s \leq 30 \quad 1 \leq N_p \leq 30 \quad 0.1 \leq a_{\text{H}_2\text{O}} \leq 3 \quad 50^\circ\text{C} \leq T_{\text{elec}} \leq 80^\circ\text{C} \quad (1)$$

To measure the system productivity, the hydrogen production will be quantified, while the Levelized Cost Of Hydrogen (LCOH) will give an indication on the system economics. To define the electrolyzer stack configuration that achieves the optimal hydrogen production and LCOH, Deterministic Design Optimization (DDO) will be performed, using the improved Nondominated Sorting Genetic Algorithm [18]. Next to the design parameters, several other technical and economic system parameters are considered (Table 1). Despite that these parameters are considered fixed in DDO, they are uncertain during real-life operation, affecting the LCOH output. To quantify the effect of these uncertainties on the output, Uncertainty Quantification (UQ) is performed. The UQ is done by non-intrusive Polynomial Chaos Expansion (PCE) [19], as this technique achieves accurate statistics in less computational time than the conventional Monte Carlo simulation technique. Moreover, PCE defines the contribution of each input parameter to the output variation through Sobol' indices, resulting in the most contributing parameters to the output variation. By using PCE to acquire the statistics, surrogate-assisted Robust Design Optimization (RDO) aims to optimize the mean and variation of the LCOH. Consequently, RDO will define a system design that achieves an LCOH that is least sensitive to uncertainties.

Table 1. The parameters, deterministic values and ranges considered in the optimization procedure.

Parameters	Deterministic value	Range
CAPEX _{PV}	780 €/kW [20]	260-1300 €/kW [20]
OPEX _{PV}	17.5 €/kW/y [20]	16-19 €/kW/y [20]
Lifetime PV, n_{PV}	25 y [20]	20-30 y [21]
CAPEX _{ELEC}	1750 €/kW [16]	1400-2100 €/kW [16]
OPEX _{ELEC}	4% [16]	3-5% [16]
Lifetime electrolyzer, n_{ELEC}	80,000 h [16]	60,000 – 100,000 h [16]
Discount rate, r	6 % [22]	2-10% [23]
Short-circuit current/temperature coefficient, μ_{isc}	0.065 A/K [24]	0.050 – 0.080 A/K [24]
Open-circuit voltage/temperature coefficient, μ_{voc}	0.080 V/K [24]	0.070 – 0.090 V/K [24]
Short-circuit current, I_{sc}	3.80 A [24]	3.79 A – 3.81 A [24]
Open-circuit voltage, V_{oc}	21.06 V [24]	21.05 – 21.07 V [24]
Diffusion current electrolyzer, i_0	1e-5 A/cm ² [4]	+/- 2% [25]
Limiting current electrolyzer, i_{lim}	2 A/cm ² [4]	+/- 2% [25]
Ambient temperature, T	climate parameter	+/- 0.5°C [17]
Solar irradiance, G	climate parameter	+/- 7% [17]
Operating temperature electrolyzer, T_{elec}	design parameter	+/- 1°C [26]
Water activity, $a_{\text{H}_2\text{O}}$	design parameter	+/- 2.5% [27]

3. Results and discussion

To illustrate the effect of the considered locations on the optimal hydrogen production and LCOH, we performed first a DDO process. By including the parameter uncertainties, we used surrogate-assisted RDO to find the design that achieves the lowest LCOH variation. To illustrate how the LCOH variation can be further reduced in this most robust design, we highlight the parameters that contribute most to the LCOH variation through UQ.

3.1. Deterministic Design Optimization (DDO) results

To achieve the optimal hydrogen production and LCOH while assuming no uncertainty on the model parameters, a multi-objective DDO has been performed. For all locations, the results show a clear trade-off between LCOH and hydrogen production (Fig. 1a,1c,1e). Clearly, Johannesburg achieves the best LCOH and hydrogen production, as it is exposed to the highest yearly solar irradiation for the compared locations. The configurations that achieve the highest hydrogen production differ in the number of parallel strings (Table 2), where the amount of parallel strings increases with the average yearly solar irradiance. To achieve a minimum LCOH, significantly fewer parallel strings are installed compared to the maximum hydrogen production designs. Due to less parallel strings in the minimum LCOH designs, the U - I characteristic slope deviates from the optimal hydrogen producing characteristic slope, resulting in a system operating out of the frequent Maximum Power Points (MPPs) (Fig. 1b,1d,1f). Therefore, lower power is transferred to the electrolyzers, resulting in a lower hydrogen production. Nevertheless, due to the reduced amount of electrolyzer units installed, the electrolyzer CAPEX is limited, resulting in the optimal LCOH eventually.

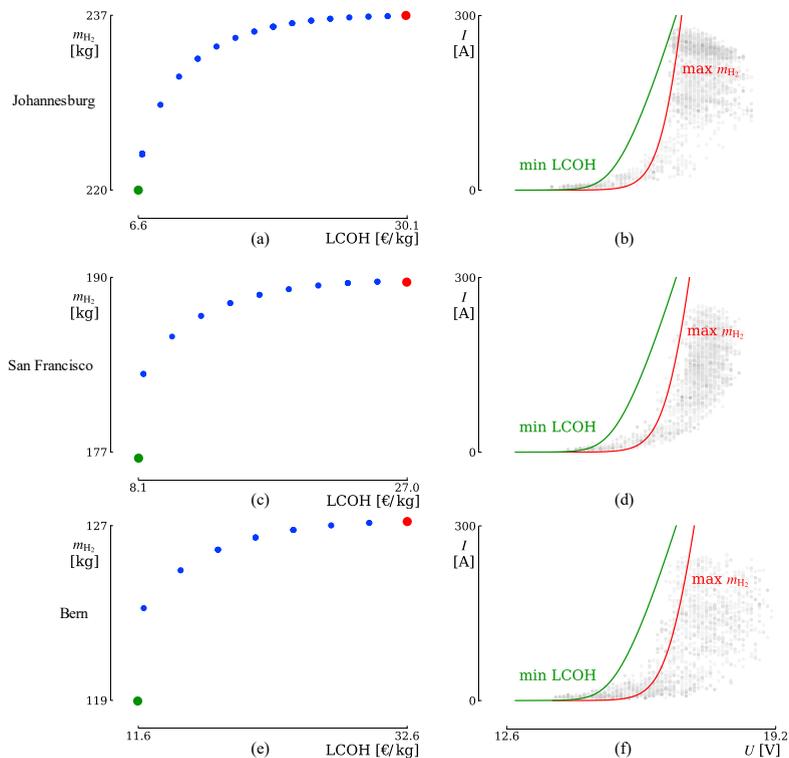


Fig. 1. A clear trade-off is visible between hydrogen production and Levelized Cost Of Hydrogen (LCOH) (a,c,e). As the electrolyzer stack configuration that achieves the minimum LCOH operates further out of the Maximum Power Points (MPPs) of the PV system (b,d,f), lower power is transferred to the electrolyzer stack, resulting in a lower hydrogen production. However, due to the reduced amount of electrolyzer units installed, the CAPEX decreases, resulting in the optimal LCOH. The grey dots in (b,d,f) correspond to the occurring of the MPPs during the year, where a white dot corresponds to not occurred, and a black dot corresponds to occurred most frequently.

Table 2. To achieve maximum hydrogen production, the number of parallel strings is the only parameter that differs over the considered locations. The number of parallel strings is significantly reduced to achieve the minimum LCOH in each location.

Location	N_s	N_p	a_{H_2O}	T_{elec} [°C]
Maximum hydrogen production				
Johannesburg	11	17	1.0	50.0
California	11	12	1.0	50.0
Bern	11	10	1.0	50.0
Minimum LCOH				
Johannesburg	10	3	1.0	50.0
California	10	3	1.0	50.0
Bern	10	3	1.0	50.0

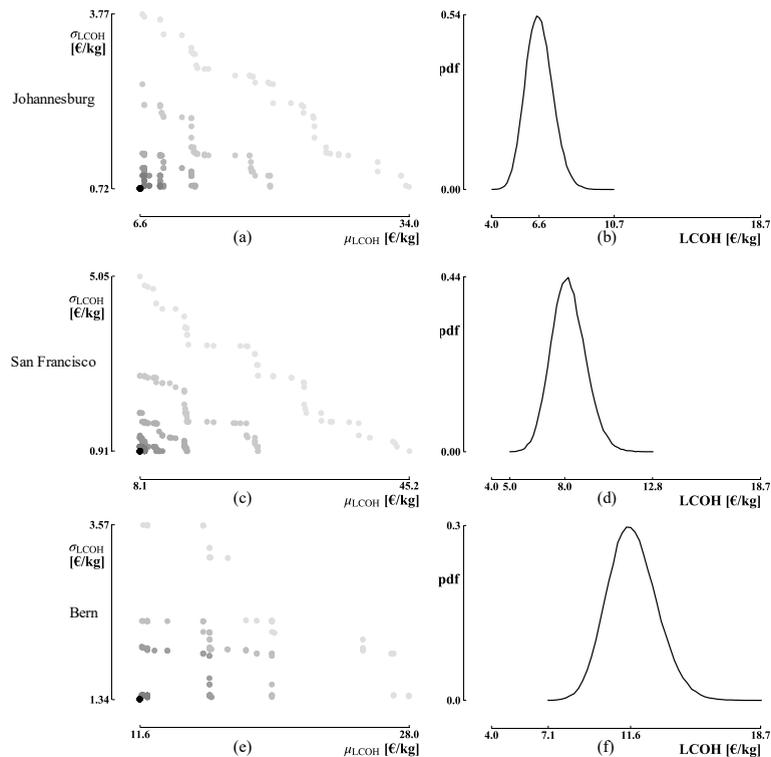


Fig. 2. For each location, the optimal LCOH mean is found at the lowest standard deviation. This means that the LCOH mean and standard deviation are non-conflicting parameters, and no Pareto front exists (a,c,e). The location with the highest average yearly solar irradiance (i.e. Johannesburg) achieves the lowest LCOH mean and standard deviation for all considered locations (b,d,f). Therefore, the PV-electrolyzer system in Johannesburg achieves the best LCOH mean with the highest probability. The grey dots in (a,c,e) present the evolution of the optimizer towards convergence, while the black dot is the converged result.

3.2. Surrogate-assisted Robust Design Optimization (RDO) results

While DDO assumes exact parameter values, the surrogate-assisted RDO algorithm considers uncertainties on the design and model parameters. The mean μ_{LCOH} and standard deviation σ_{LCOH} for the LCOH is determined using PCE for each stochastic design sample. Based on these statistics, the optimizer looks for a design sample that minimizes both objectives (or a Pareto set of design samples when the objectives are conflicting). When convergence is reached, μ_{LCOH} and σ_{LCOH} appear to be non-conflicting objectives. As a result, the most robust design achieves the optimal mean

LCOH as well (Fig 2a,2c,2e). When comparing the locations, Johannesburg achieves the lowest μ_{LCOH} equal to 6.6 €/kg, with the lowest σ_{LCOH} of 0.72 €/kg (Fig. 2b,2d,2f). Therefore, installing a PV-electrolyzer system in locations with a high average yearly solar irradiation is favorable for both the mean and standard deviation of LCOH.

3.3. Uncertainty Quantification (UQ) results

While the surrogate-assisted RDO process delivers the design that is least sensitive to uncertainties, Uncertainty Quantification (UQ) is used to provide the contribution of each input parameter to the LCOH variation. To achieve accurate statistics at a tolerable computational cost, Polynomial Chaos Expansion (PCE) is used in the UQ process. Compared to a reference result achieved by Monte Carlo Simulation, a PCE order of 3 achieves moments with an error below 0.01% on the mean and 0.1% on the variance. When applied to the most robust design, the Sobol' indices illustrate the contribution of each parameter to the LCOH variation. Clearly, the discount rate r and CAPEX parameters are the main parameters inducing the LCOH variation (Fig. 3). Therefore, restricting the discount rate range, by de-risking the technology or having more demonstrating projects, is concluded to be the most significant action to further reduce the LCOH variation in the most robust design.

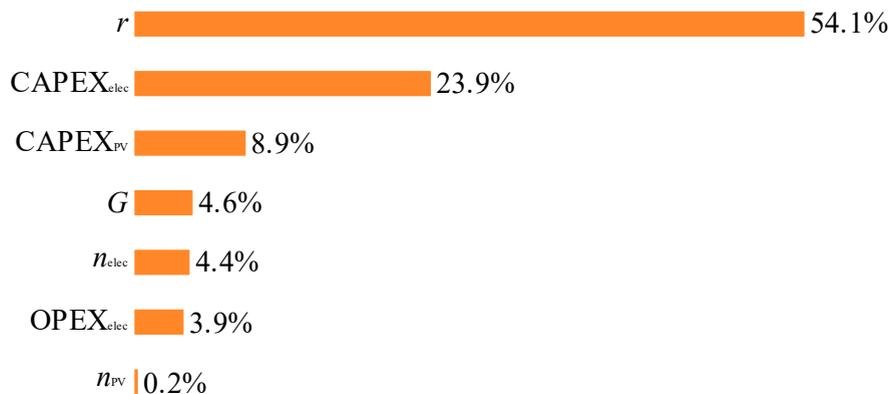


Fig. 3. The Sobol' indices indicate that the LCOH variation is mainly dominated by the discount rate r and CAPEX parameters.

4. Conclusion

PV systems need energy carriers to comply with the time-flexible energy demand. By combining a PV-system with an electrolyzer stack, a viable storage system is provided. Optimizing the electrolyzer stack configuration in terms of hydrogen production and LCOH results in a Pareto set of optimal solutions. The location with the highest average yearly solar irradiance results in the optimal hydrogen production or LCOH. When including the model parameter uncertainties, the surrogate-assisted RDO results show that the LCOH mean and standard deviation are non-conflicting parameters. Moreover, the location with the highest average yearly solar irradiance results in the minimum LCOH mean (6.6 €/kg) and standard deviation (0.72 €/kg). Therefore, installing a PV-electrolyzer system in locations with a high average yearly solar irradiation is favorable for both the mean and standard deviation of LCOH. When analyzing the contribution of each system parameter individually to the LCOH variation of the most robust design, the UQ process demonstrated the major contribution of the discount rate. Therefore, de-risking the technology or promoting more demonstration projects is the main action to further decrease the LCOH variation. Future works will focus on including accurate probability distributions and adding batteries to the system.

Acknowledgements

The work has been performed in the scope of the GenComm project, funded by Interreg North-West Europe.

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