

Electrochemical conversion technologies for optimal design of decentralized multi-energy systems: Modeling framework and technology assessment[☆]



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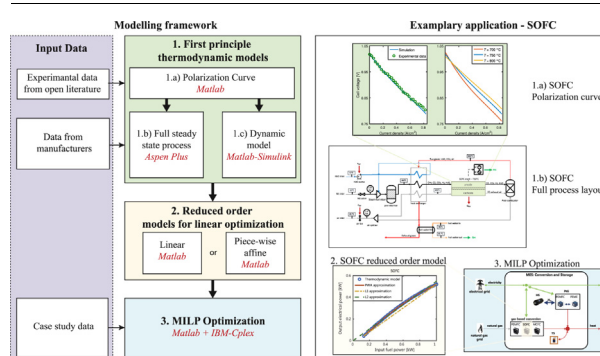
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HIGHLIGHTS

- Accurate linear models derived from first-principle thermoelectric models.
- Suitable level of details for technology simulation within integrated systems.
- Critical techno-economic parameters for fuel cell distributed cogeneration.
- Dynamics and electrical-to-thermal efficiency crucial for modeling and application.
- Design principles for fuel cell-based distributed cogeneration.

GRAPHICAL ABSTRACT



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ABSTRACT

The design and operation of integrated multi-energy systems require models that adequately describe the behavior of conversion and storage technologies. Typically, linear conversion performance or fixed data from technology manufacturers are employed, especially for new or advanced technologies. This contribution provides a new modeling framework for electrochemical devices, that bridges first-principles models to their simplified implementation in the optimization routine. First, thermodynamic models are implemented to determine the on/off-design performance and dynamic behavior of different types of fuel cells and of electrolyzers. Then, as such nonlinear models are intractable for use in the optimization of integrated systems, different linear approximations are developed. The proposed strategies for the synthesis of reduced order models are compared to assess the impact of modeling approximations on the optimal design of multi-energy systems including fuel cells and electrolyzers. This allows to determine the most suitable level of detail for modeling the underlying electrochemical technologies from an integrated system perspective. It is found that the approximation methodology affects both the design and operation of the system, with a significant effect on system costs and violation of the thermal energy demand. Finally, the optimization and technology modeling framework is exploited to determine guidelines for the installation of the most suitable fuel cell technology in decentralized multi-energy systems. We show how the installation costs of PEMFC, SOFC and MCFC, their electrical and thermal efficiencies, their conversion dynamics, and the electricity price affect the system design and technology selection.

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1. Introduction

During the 20th century, the energy industry succeeded in the difficult task of meeting the rising electricity and heat demand, which was driven by growing populations and economies. Indeed, this was possible thanks to the use of fossil fuels in large-scale centralized plants, which supply power through national and international transmission and distribution grids. However, the evidence that the anthropogenic alteration of the earth carbon balance is leading to climate change has triggered the necessity of finding new routes for energy provision, where no-carbon emission is a must-have feature. In this context, energy efficiency and renewables are the most important building blocks of a pathway consistent with the COP 21 goal of keeping global warming “well below” 2 °C [1]. It is well recognized by both institutional bodies and private organizations, that distributed energy technologies represent a key enabler of these measures, as they open significant opportunities to reduce carbon emissions and improve efficiency, while keeping the costs limited, and retaining system reliability [2–7]. As a result, both the energy market and infrastructures are being transformed by the development of decentralized energy systems. Especially, the benefits of going decentralized on the energy efficiency and renewable penetration are maximized when multi-energy systems (MES), which exploit the interaction between different energy carriers (e.g. electricity, natural gas and heat), are adopted [8]. On the other hand, the complexity of such systems, which is largely dependent on (i) the number of technologies that can be combined, (ii) the different operation modes that can be adopted, (iii) the uncertainty linked to non-dispatchable generation (i.e. PV and wind) and energy demands, and (iv) the topology of multiple MES integrated with the distribution grid, make the design and operation of such systems particularly challenging. As a consequence, this has prompted many researchers to develop algorithms and computer tools that can tackle such problem. For an overview of the relevant activity in the field, readers are referred to the works by Keirstead et al. [9] and Allegrini et al. [10], who reviewed simulation models within the framework of distributed multi-energy systems. In particular, mixed-integer linear programming (MILP) has been particularly favored as optimization method to design and operate multi-energy systems thanks to its flexibility in reproducing complex systems while keeping the computational effort limited. Accordingly, the number of works on this topic is significant. Relevant analyses focused on the optimal sizing and operation of the energy system (e.g. [11–17]), on the multi-objective nature of the problem (see e.g. [18–21]), and on energy networks (see e.g. [13,22–26]). Along with this, but in a limited number of examples, experimental tests research is carried out (e.g. [27]). However, in the majority of aforementioned works a simplified description of the technology conversion performance is implemented, which neglects the change of the performance with the size and the partial-load operation. Moreover, the dynamics of the conversion technologies is often limited to the start-up/shut-down or minimum run-time (e.g. [13,28]). The reasons behind this simplified approach lie in the complexity of the optimization problem, but also in the lack of a bridge between the research at the technology/process level and the research on optimization of MES. This has hindered the adoption of models, more or less detailed, for the conversion technologies, which are in most of the works represented with a constant efficiency in the matrix of coefficients, or, in a few cases, by a set of given efficiencies for part load operation (the description and formulation of the input/output relationships in an energy hub via matrix modeling, with and without constant efficiency, is comprehensively reported in Chicco and Mancarella [29] and Mancarella et al. [30]). Notably, an alternative approach to the constant efficiency formulation was already described by Bloomfield and Fisk in their pioneering work of 1981 [31], where they adopted a piecewise function for the description of heat pumps in a linear optimization problem. More recently, a number of researchers started to tackle this problem within the energy hub framework: Salgado and Pedrero showed how the

performance of a combined heat and power (CHP) plant, where the heat and electric output are not independent, can be formulated within an MILP problem [32]; Evins et al. have adopted an improved version of the Bloomfield and Fisk’s algorithm for better description of heat pumps operating at partial load [28]; Zhou et al. studied the impact of off-design performance of boilers and engines on the optimal design and operation of combined cooling, heating and power systems [33]; Bischi et al. developed a piecewise affine approximation for modeling the partial-load performance of the conversion units (boilers, heat pumps and refrigerators) in a MILP [34]; Bracco et al. distinguished between two different values for the maximum and rated efficiencies of some conversion units [35]; Finally, Milan et al. investigated the nonlinear performance of fuel cells, micro-turbines, and internal combustion engines within a MILP [36].

In the framework of multi-energy systems, electrochemical conversion technologies, namely fuel cells and electrolyzers, are regarded as key elements of the technology portfolio. On the one hand, fuel cells (FC) are electrochemical devices that allow for co-generating electricity and heat with very high electrical efficiency regardless of the technology size. Moreover, thanks to their modularity and to the different types of electrolytes that can be adopted, FC can be deployed both at micro and large scale (i.e. kW and MW scale, respectively) without affecting the performance significantly. On the other hand, electrolyzers, which generate hydrogen and oxygen by absorbing electric power through the splitting of deionized water, constitute one of the few technologies that enable seasonal storage of energy with limited (virtually zero) losses of energy over time. Despite the vast research on the use of electrochemical devices in multi-energy systems, there is no clear framework for a reliable description of these technologies in the formulation of such optimization problems. Fuel cells and electrolyzers are either described with constant performance [15,20,37] or as black box models based on manufacturer or literature data [36,38,39]. In all cases, the performance is not clearly connected to first principle thermodynamic models. This is particularly important whenever an integrated system perspective is adopted to provide guidelines for the development of new devices or to compare different fuel cells.

With this contribution we want to overcome these shortcomings, and in particular we aim at (i) providing a clear methodology for the computation within MES optimization problems of realistic electrochemical performance, which are based on first principle models and which can be tuned for whatever electrochemical device; (ii) providing reliable reduced order models for simulating electrochemical devices within the optimization framework, that can be easily implemented in future research works; (iii) assessing the impact of various modeling approximations on the optimal design of integrated multi-energy systems that include electrochemical devices, i.e. determining the most suitable level of detail for simulating these technologies from an integrated system perspective; (iv) making use of these new tools to identify key guidelines for the adoption of different fuel cells in multi-energy systems. To this end, first-principle models are implemented to determine the performance of different electrochemical devices under various operating conditions. These are then linearized using different approaches and implemented in the MILP formulation. The optimization framework presented in [40] is adopted to evaluate the impact of approximate conversion efficiency and conversion dynamics on the minimum-cost design of the integrated system. The methodology presented in this work has been applied to the main commercial electrochemical devices, including: proton exchange membrane fuel cells (PEMFC), solid oxide fuel cells (SOFC), molten carbonate fuel cells (MCFC) and polymer membrane electrolyzers (PEME). Note that this methodology can be easily applied to electrochemical technologies not included in this work and holds when considering different objective functions of the optimization problem (e.g. minimum CO₂ emissions). The modeling framework for electrochemical devices presented in details in this work has recently been adopted by Murray et al. [41], and Gabrielli et al. [40].

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