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Optimization of hydrogen yield of a high-temperature electrolysis system with coordinated temperature and feed factors at various loading conditions: A model-based study☆

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HIGHLIGHTS

- Describe an operating system with energy flows.
- An analytical optimization model to operate a plant.
- Conversion efficiency and load range increased.
- More hydrogen yield from fluctuant surplus power.

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ABSTRACT

High-temperature electrolysis (HTE) is a promising technology for achieving high-efficiency power-to-gas, which mitigates the renewable curtailment while promoting decarbonization by transforming wind or solar energy into fuels. Different from low -temperature electrolysis, a considerable amount of the input energy is consumed by auxiliary equipment in an HTE system for maintaining the temperature, so the studies on systematic energy description and parameter optimization of HTE are essentially required. A few published studies investigated HTE's systematic optimization based on simulation, yet there is not a commonly used analytical optimization model which is more suitable for integration with power grid. To fill in this blank, a concise analytical operation model is proposed in this paper to coordinate the necessary power consumptions of auxiliaries under various loading conditions of an HTE system. First, this paper develops a comprehensive energy flow model for an HTE system based on the fundamentals extracted from the existing work, providing a quantitative description of the impacts of condition parameters, including the temperature and the feedstock flow rates. A concise operation model is then analytically proposed to search for the optimal operating states that maximize the hydrogen yield while meeting the desired system loading power by coordinating the temperature, the feedstock flows and the electrolysis current. The evaluation of system performance and the consideration of constraints caused by energy balances and necessary stack requirements are both included. In addition, analytical optimality conditions are obtained to locate the optimal operating states without performing nonlinear programming by further investigating the optimization method. In the case study, a numerical case of an HTE system is employed to validate the proposed operation model and optimization method, which proves that the proposed operation strategies not only improve the overall conversion efficiency but also significantly enlarge the load range of the HTE system. A 24-h case with fluctuant power input is also simulated to validate the beneficial effects of the proposed operation strategies on producing more hydrogen from a specific profile of surplus electricity. At last, some results comparisons with existed papers and possible research extensions are discussed briefly.

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Nomenclature

Chemical thermodynamics and kinetics

Γ	pre-exponential factor
σ	electrical conductivity
ξ	activation energy
c	isobaric specific heat capacity
C_T	isobaric molar heat capacity at temperature T
F	Faraday constant
$G_{T,\tilde{\boldsymbol{p}}}$	molar Gibbs free energy at condition (T, $\tilde{\boldsymbol{p}}$)
h	specific enthalpy
H_T	molar enthalpy at temperature T
M	molar mass
n_e	number of electron exchanges. For (1), $n_e = 2$
p	pressure
R	molar gas constant
$S_{T,\tilde{\boldsymbol{p}}}$	molar entropy at condition (T, $\tilde{\boldsymbol{p}}$)
T	temperature
T_H	reference point around operating temperature
T_L	reference point around ambient temperature

Notations

$\bar{X}$	$\frac{1}{l_{s4}-l_{s3}}\int_{s3}^{s4} X \mathrm{d}l$
$\Delta_r X$	$X_{H_2} + X_{O_2} - 0.5X_{H_2O}$
$\tilde{\boldsymbol{p}}$	$[p_{H_2O} \quad p_{H_2} \quad p_{O_2} \quad p_{N_2}]^T$
$\tilde{\boldsymbol{w}}$, $\tilde{\boldsymbol{\pi}}$	$[w_{ca} \quad w_{an}]^T$, $[\pi_{ca} \quad \pi_{an}]^T$
$\widehat{X}$	$(w_{ca}X_{ca} + w_{an}X_{an})/(w_{ca} + w_{an})$
$\mathrm{mix}_{an}(X)$	$(p_{O_2}X_{O_2} + p_{N_2}X_{N_2})/(p_{O_2}M_{O_2} + p_{N_2}M_{N_2})$

Operation variables

χ	molar fraction
η	efficiency
ω	mass fraction
π	feed factor
ρ	mass density
OP	operating points
I	direct current
i	current density
L	geometric length
P	power
U	(equivalent) voltage or overvoltage
v	flow velocity of gas mixture
w	mass flow rate of gas mixture

Superscript and subscripts

$\ominus$	standard state, i.e., pressure at $p^\ominus$ for gases
act, con, ohm	activation, concentration, ohmic (overvoltage)
ca, ele, an	cathode, electrolyte, anode
cha, cel, sys	channel, cell, system
el, ex	electrolysis, exchange (current density)
fur, com	furnace, compressor
pum, pre	pump group, preheater
rea, war, dis	reaction, warming, heat dissipation
rev, th	reversible, thermo-neutral (voltage)
s0, ...,s4	at cross section 0,…,4 shown in Figs. 1 and 4
vap, liq, amb	vaporization, liquid, ambient
x, y, z, l	spatial dimensions

1. Introduction

The integration of renewable generation sources is faced with formidable challenges because of their undesirable intermittence caused by uncontrollable factors [1]. By producing fuel gases with fluctuating electricity and storing the renewable energy that may otherwise be curtailed, the power-to-gas (P2G) approach presents an attractive solution for meeting the increasing energy demand in an ecofriendly manner [2,3]. Moreover, P2G plays an important role in the context of multi-energy systems by functioning as the interaction points to couple the gas network and the power system [4]. Numerous P2G pilot systems have been constructed around the world for research or demonstration purposes as seen in [5,6]. Actually, it is reported that the levelized fuel cost of P2G is potentially competitive to the prices of diesel and natural gas by 2020 [7], and it will not be long before a profitable plant is presented.

Plenty of studies on P2G's operation and dispatch in the energy supply system have been conducted, such as [8–10], which validated the benefits on energy decarbonization and renewable integration from massive implementation of P2G-based energy storage in the future. However, these studies mostly treated the P2G systems as simple electricity-gas correlation nodes with fixed conversion efficiencies and simple capacity limits, regardless of their inherent model complexities or local control, such as the P2G process modeling in [11], which in turn limits the accuracy and practicability of these studies. To improve this situation, we also need to dig inside of the P2G systems to consider their internal constraints and operating strategies.

Inside a P2G system, the energy conversion is based on the electrolysis process, where H_2O splits into H_2, which can be further converted into CH_4 with an optional methanation reactor [12,13]. Conventionally, the electrolysis occurs below 100 °C when using liquid water with the help of an alkaline solution or a polymer electrolyte membrane. Regarding the mass production of hydrogen, however, high-temperature electrolysis (HTE) is a more promising technology because of its advantage of a substantially higher potential efficiency as described in [12,14,15]. With vaporous feedstock and a solid oxide electrolyte, HTE can achieve a much lower electrolysis voltage by providing an elevated temperature that aids the reaction both kinetically and thermodynamically [16]. In contrast to low-temperature electrolysis systems based on alkaline or polymer electrolyte membrane electrolyzers, a significant fraction of the overall energy consumption is attributed to the auxiliaries in an HTE system, particularly for heating purposes [17,18].

As mentioned before, a full investigation inside the HTE system is required for its further implementation in existing power systems and its integration with renewable energy facilities. The fundamentals of this topic are internal characteristics of HTE stack, such as electrolysis theories, cell models and stack configurations. These points have long been well supported by many published works. A one-dimensional HTE model considering overvoltages and internal balances was developed by [16] for steady-state evaluation at various temperatures and current densities. Reference [19] presented a dynamic cell model of a planar solid oxide cell in electrolytic mode (i.e., HTE) and then performed model validation using the available experimental results. Reference [20] employed a computational fluid dynamics approach to model a cross-flow solid oxide electrolysis cell and then obtained the three-dimensional profiles of current density, temperature, and hydrogen's molar fraction via finite volume method. Reference [21] simply modeled the solid oxide electrolyzer as an electrical-chemical-heat energy equilibrium coupling with ammonia synthesis process for hydrogen