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Low-temperature electrolysis system modelling: A review

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ABSTRACT

This review provides an exhaustive and comprehensive analysis of the existing modelling works about low temperature electrolysis system: alkaline and proton exchange membrane (PEM) technologies. In order to achieve this review, a classification was built, based on different criteria such as physical domains involved or modelling approaches. The proposed methodology allows both exposing an overview of the electrolysis system modelling field and providing a deep analysis of each reviewed model. Actual strengths, weaknesses and lacks in this research field are pointed out and the performed analysis provides ideas for future research in this area.

1. Introduction

In 21th century, humankind has to cope with one of its biggest challenge: mitigate greenhouse gas emissions to limit climate change while supplying increasing energy demand to favor economic growth [1]. Within this framework, hydrogen-energy appears as a good way to facilitate the transition towards a low-carbon society [2–5]. Indeed, hydrogen has a high energetic density and its utilization does not cause any pollutant emission. Its wide range of uses [6–8] especially as a fuel for mobility make it a good alternative to fossil energy [7].

Otherwise, the penetration of renewable sources on the European electricity network involves the probability increase of supply and demand mismatching occurrence [9,10]. Connecting an intermittent electric source to an electrolyser system to produce hydrogen is then a good way to convert and store the electrical energy excess [11]. Besides, water electrolysis technology is one of the current leading technologies for producing low carbon hydrogen as long as the electrolysis system is fed with low carbon electricity [12–16]. Therefore, electrolysis enables to solve both issues: large scale production of green hydrogen and electrical energy storage.

In order to face the dynamic issues of connecting an intermittent electrical source to an electrolysis system, modelling is a critical and powerful tool for phenomena understanding, control analysis, sizing, energy management and optimisation. The purpose of this work is to present an exhaustive and comprehensive review of existing works about low-temperature electrolysis system modelling that have been developed in the literature. Some electrolysis modelling reviews such as the ones included in [17–21] can be found, but these ones are only focused on several modelling works. Therefore, this paper enables to present an overview on this topic in order to identify the actual strengths and weakness of existing research and offer orientations to future works.

It is organized as follows. After this brief introduction, the second section is dedicated to a description of electrolysis technology, the interest for modelling and the presentation of the methodology used in order to analyse the models reviewed. The third part deals with an exhaustive presentation of consulted papers based on a classification of different types of models. Finally, the fourth section draws a synthesis of the reviewed models and the associated modelling approaches, and proposes ideas for future research in this area.

2. Electrolysis modelling and associated issues

2.1. Electrolysis technology presentation

The water electrolysis reaction is achieved in an electrolysis cell composed of: (i) an electrolyte (ionic conductor), (ii) active layers at which the redox reactions occur and (iii) current and materials collectors (electronic conductor) enabling the electricity supply and the supply and collection of reagents and products.

This paper is focused on alkaline and proton exchange membrane electrolysis systems modelling. These low-temperature technologies are well-matured [17,22–26] (compared to high temperature electrolysis) and they have already been integrated in some industrial-scale projects in order to demonstrate their abilities to convert intermittent electric sources into hydrogen [8]. The operating principle of alkaline and PEM technologies are exposed in the Fig. 1.

In order to produce hydrogen at large scale, cells are assembled into

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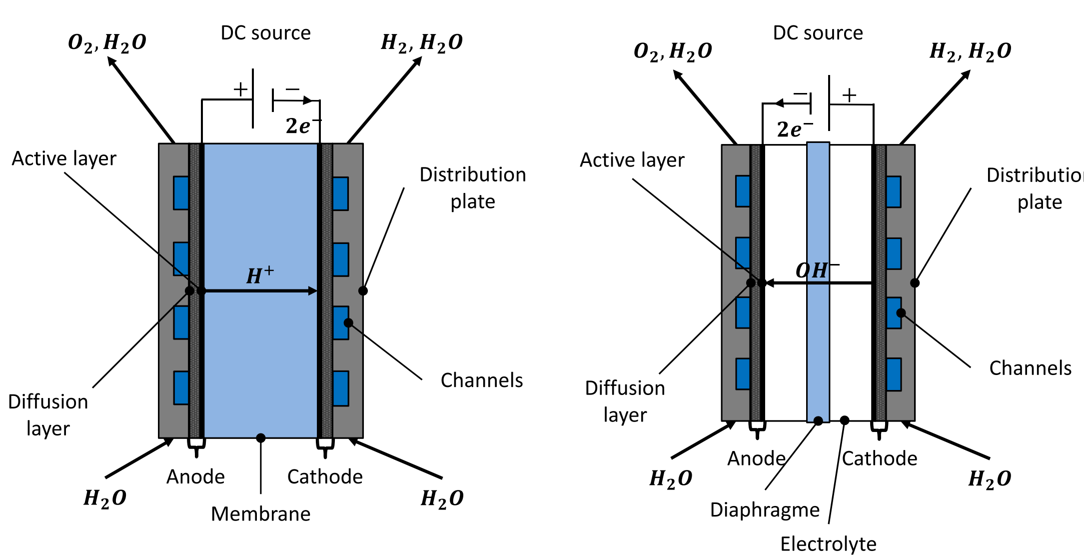
Nomenclature

$I_{0,k}$	current exchange density at electrode k (A m^{-2})
α_k	charge transfer coefficient at electrode k
z	number of electrons involved in the reaction
U_{tn}	thermoneutral voltage (V)
η_{far}	Faraday efficiency
σ_{PEM}	proton exchange membrane conductivity (S m^{-1})
λ	water content of the membrane
$\sigma_{alkaline}$	alkaline electrolyte conductivity (S m^{-1})
$\dot{\eta}_{eos}$	electro-osmosis flow (mol s^{-1})
η_{eos}	electro-osmosis coefficient
A	electrolysis cells area (m^2)
L	proton exchange membrane length (m)
F	Faraday constant (C mol^{-1})
T	cell(s)/stack(s) Temperature (K)
R	ideal gas constant (J mol^{-1} K^{-1})
C_{PE}	products concentration near electrode (mol m^{-3})
C_{PS}	products concentration in the solution (mol m^{-3})
C_{RE}	reagents concentration near electrode (mol m^{-3})
C_{RS}	reagents concentration in the solution (mol m^{-3})
w	mass concentration of alkaline electrolyte (wt%)
m	molar concentration of alkaline electrolyte (mol m^{-3})
θ	covering coefficient
σ_{free}	electrolyte conductivity free of bubbles (S m^{-1})
σ_e	bubbles-corrected electrolyte conductivity (S m^{-1})
C_{stack}	thermal capacitance of the stack (J K^{-1})
We	electrical work (W)
$\dot{Q}$	heat flow (W)
A_r	chemical affinity of the water dissociation reaction (J mol^{-1})
μ_i^0	standard chemical potential of species i (J mol^{-1})
μ_i	chemical potential of species i (J mol^{-1})
μ_i^*	electrochemical potential of species i (J mol^{-1})
ΔrH	enthalpy of water dissociation reaction (J mol^{-1})
ΔrG	free enthalpy of water dissociation reaction (J mol^{-1})
ΔrS	entropy of water dissociation reaction (J K^{-1} mol^{-1})
ν_i	stoichiometry coefficient of species i in water dissociation reaction
η	converter efficiency (%)
η_{10}	converter efficiency at 10% of its nominal power (%)
η_{100}	converter efficiency at nominal power (%)
P_{nom}	converter nominal power (W)
P_s	converter output power (W)
I	stack current (A)
J	stack density current (A m^{-2})
E_{cell}	cell voltage (V)
E_{rev}^0	standard reversible potential (V)
E_{rev}	reversible potential (V)
$E_{act,ano}$	anode activation overvoltage (V)
$E_{act,cat}$	cathode activation overvoltage (V)
E_{ohm}	ohmic overvoltage (V)
E_{diff}	diffusion overvoltage (V)
D_i	diffusion coefficient of species I (m^2 s^{-1})
H_i	Henry constant of species i (m^3 Pa mol^{-1})
$\dot{n}_i$	molar flow of species i (mol s^{-1})
n_i	partial pressure of species i (Pa)
P_i	partial pressure of species i (Pa)
a_i	chemical activity of species i
Cp_i	molar thermal capacitance of species i (J K^{-1} mol^{-1})
$[i]$	concentration of species i (mol m^{-3})
ρ_i	density of species i (kg m^{-3})
K_i	permeability coefficient of species i (m s^{-1})
M_i	molar mass of species i (kg mol^{-1})

a stack by the mean of bipolar plates. These ones contain channels in order to feed the cell with reagents and evacuate the gases produced. An electrolysis stack is then an assembly of numerous open electrochemical reactors. In order to ensure the good operation of these reactors, several functions are required and cannot be accomplished by the stack on its own. That is why an electrolysis system must include auxiliary components in order to carry out:



Anode	$H_2O \rightarrow \frac{1}{2}O_2 + 2H^+ + 2e^-$	$2H_2O + 2e^- \rightarrow 2OH^- + H_2$	**Anode**
Cathode	$2H^+ + 2e^- \rightarrow H_2$	$2OH^- \rightarrow \frac{1}{2}O_2 + H_2O + 2e^-$	**Cathode**
Total reaction	$H_2O \rightarrow \frac{1}{2}O_2 + H_2$	$H_2O \rightarrow \frac{1}{2}O_2 + H_2$	**Total reaction**

Fig. 1. Schematic of the operating principle of an alkaline and PEM water electrolysis cell.

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