ABSTRACT
In this research paper, a solar based hydrogen production is considered for the city of Tehran, the capital of Iran. Photovoltaic panels (PV) are used for electricity generation and they connect to polymer electrode membrane (PEM) electrolysis for hydrogen production. TRNSYS software is used for the weather data in Tehran and PV panel simulation. Since the system is a dynamic one, a 1D dynamic fluid flow model is used to simulate a PEM electrolyzer cell. Output solar power during a typical year is imposed on the electrolyzer and the performance of the system is investigated. In this regards, high pressure and atmospheric water electrolysis is compared. The results shows that although high pressure electrolysis reduced compressor work, for integrated system atmospheric electrolysis has higher efficiency.

NOMENCLATURE
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tr>
<td>C</td>
<td>concentration</td>
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<tr>
<td>D_{w}</td>
<td>water diffusion coefficient in membrane</td>
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<td>E</td>
<td>Open circuit voltage</td>
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<td>F</td>
<td>Faraday constant</td>
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<td>G</td>
<td>Cell irradiance</td>
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<td>h_{m}</td>
<td>membrane thickness</td>
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<td>i</td>
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<td>anode exchange current density</td>
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<td>i_{cn}</td>
<td>cathode exchange current density</td>
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<td>K</td>
<td>Darcy’s constant</td>
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<td>n_{ed}</td>
<td>electro-osmotic drag coefficient</td>
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<td>P</td>
<td>Pressure</td>
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<td>gas universal constant</td>
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<td>electrical resistance</td>
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<td>Temperature</td>
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<td>u</td>
<td>velocity</td>
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<td>Cell voltage</td>
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<td>Gibbs free energy of formation</td>
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<td>membrane conductivity</td>
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<td>Ohmic over-potential</td>
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<tr>
<td>\eta_{an}</td>
<td>Anodic activation overpotential</td>
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<tr>
<td>\eta_{cn}</td>
<td>Cathodic activation overpotential</td>
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<tr>
<td>\lambda_{m}</td>
<td>membrane humidification</td>
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<td>\rho</td>
<td>Density</td>
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1-INTRODUCTION
Energy use is directly linked to well-being and prosperity across the world. Meeting the growing demand for energy in a safe and environmentally responsible manner is an important challenge. A key driver of energy demand is the human desire to sustain and improve ourselves, our families and our communities. There are around seven billion people on Earth and population growth will likely lead to an increase in energy demand, which depends on the adequacy of energy resources. In addition, increasing population and economic development in many countries have serious implications for the environment, because energy generation processes (e.g., generation of electricity, heating, cooling, and shaft work for transportation and other applications) emit pollutants, many of which are
harmful to ecosystems. Burning fossil fuels results in the release of large amounts of greenhouse gases, particularly carbon dioxide [1]. In recent years, focusing on global CO2 reduction, and searching for non-emission sustainable technologies have substantially increased. Among various renewable energy sources, solar and wind energy are expected to have major role in future of energy market as well as hydrogen as an energy carrier [1]. Water electrolysis can efficiently convert clean energy sources into hydrogen and is the most mature technology in for near future term [2]. Electrolyzers are unique devices to produce pure hydrogen and oxygen which can be used for later applications such as fuel for hydrogen cars and as an storage media. They could be widely distributed and rated to meet the hydrogen and oxygen requirements of different users such as units for individuals, renewable energy systems, fueling stations and industrial applications [3].

PEM electrolysis is one of the applicable and efficient methods and many researches have focused on the state-of-the-art to make it widely cost effective for different applications. PEM electrolyzer comparing to other technologies has several advantages such as higher efficiency, higher current density toleration, pure gas production and safer operation which is the result of not using hazardous liquid electrolyte. They can independently produce high pressure hydrogen which somehow could reach up to 130 bar [4] which is beneficial from economical point of view [2-8].

Electrolyzer modeling has been a subject of many researches and they presented simple thermodynamic model to more sophisticated ones. In this regards, Gorgun [3] developed a dynamic model based on conservation of mole balance at the anode and the cathode. Dale et. al. [9] peresented a semi practical model and considered a temperature dependency of reversible voltage. They use curve-fitting method for fitting the experimental data and determining model parameters. Santarelli et. al. [5] investigated the effect of temperature, pressure and feed water flow rate on electrolyzer performance using a regression model. Marangio et. al. [10] proposed a theoretical model of electrolyzer system consisting of activation, concentration and ohmic overpotentials. Awasthi et. al. [11] developed a dynamic model in MATLAB/Simulink with the ability to investigate the effects of various operating condition and electrolyzer components. Lee et. al. [12] represented a dynamic model of PEM electrolyzer for regenerative fuel cell applications. They investigated the effects of temperature and mass flow rate and validated their model with experimental data. Kim et. al.[1] developed a one-dimensional dynamic model of a high-pressure PEM water electrolyzer. Water transport, gas permeation, gas volume variation in anode/cathode channels, gas compressibility, and water vaporization are considered in their model. In this research paper, we proposed a new one dimensional (1D) dynamic model which is useful for system applications due to capability of selecting larger time step and lower mesh nodes. The proposed model is used to evaluate dynamic behavior of a PEM electrolyzer imposed on typical yearly solar power generated from photovoltaic panels which is located in Tehran. TRNSYS software is used for the weather data in Tehran and PV panel simulation.

2-ELECTROLYZER MODELING

Fig.1 shows the schematic of a PEM water electrolyzer in which the electrolyzer cell divided into three segments namely anode channel,
cathode channel and membrane electrode assembly (MEA). Water from anode channel diffuses to MEA and there decomposed to proton and oxygen. Protons migrate through membrane and compound with the electrons supplied from DC source to produce hydrogen in the cathode electrode.

![Fig.1: Schematic of a PEM electrolyzer cell](image)

2-1-ELECTROCHEMICAL EQUATIONS

The voltage required to overcome the water molecule link in the PEM cell is given by eq.1:

\[ V = E_0 + \eta_{ohm} + \eta_{an} + \eta_{cat} \]  

Where \( V \) is the electrolyzer voltage and \( \eta_{ohm}, \eta_{an}, \) and \( \eta_{cat} \) are ohmic, anode activation and cathode activation overpotentials respectively. \( E_0 \) is open circuit voltage which can be edetermined from the Nernst equation (eq.2) [13]:

\[ E = E_0 + \frac{RT_e}{2F} \ln \left( \frac{P_{H_2}^2}{P_{H_2O}} \right) \]  

Where \( E_0 \) is the standard potential, \( R \) is the gas universal constant, \( T_e \) is the cell temperature and \( a_{H_2O} \) is the activity of water between anode and electrode that can be assumed equal to 1 for liquid state. The standard potential is calculated from eq.3 [13]

\[ E_0 = \frac{\Delta G_f}{2F} \]  

Where \( \Delta G_f \) is the Gibbs free energy of formation.

Ohmic overpotential in the PEM electrolyzer occurs due to electrical resistance of the cell against the electrical current and membrane resistance against proton migration. This over-potential can be formulated as below (eq.4) [1]:

\[ \eta_{ohm} = \eta_{an} + \eta_{cat} \frac{1}{\sigma_{mem}} \]  

In the eq.2 \( \tau_{an}, \tau_{mem} \) and \( \sigma_{mem} \) are the cell electrical resistance, the membrane thickness and the conductivity of membrane respectively. Here, we assumed that electrodes are perfect conductors so voltage is constant throughout them [1]. Membrane conductivity depends on water content and temperature of membrane which can be estimated from below (eq.5) practical equation [10].

\[ \sigma_{mem} = \left[ 0.025 \times 10^{-3} \times \exp \left( \frac{T}{298} \right) \right] \]  

Activation over-potential is obtained from simplified form of Butler-Volmer equation [10]

\[ \eta_{an} = \frac{RT_e}{2F} \ln \left( \frac{i}{i_{an,0}} \right) \]  

\[ \eta_{cat} = \frac{2RT_e}{F} \ln \left( \frac{i}{i_{cat,0}} \right) \]  

\( F \) is faraday constant, \( i_{an} \) and \( i_{cat} \) are exchange current densities at anode and cathode respectively. Production/destruction species rate is given by Faraday's law:

\[ \eta_{an} = \frac{1}{2F} \]  

\[ \eta_{cat} = \frac{i}{4F} \]  

2-2-WATER TRANSPORT MECHANISMS

Three major water transport mechanisms exist in the PEM electrolyzer cell consisting of concentration gradient, pressure gradient and electro-osmotic drag.
Among them, the last one has the most important role in water transportation [1,10,11]. Water transport due to concentration gradient is obtained using Fick's law [14]

\[ n_a = D_w \frac{C_{Wi} - C_{Wa}}{h_{mem}} \]  (11)

where \( D_w \) is the water diffusion coefficient in membrane, \( h_{mem} \) is membrane thickness, \( C_{Wi} \) and \( C_{Wa} \) are water concentration at cathode side and anode side respectively. Water transport due to pressure gradient can be calculated using Darcy's law [14]:

\[ n_p = \left( \frac{K_{D,w} \rho_w}{\mu_w} \right) \frac{P_c - P_a}{h_{mem}} \]  (12)

Where \( K \) is the Darcy constant, and \( \rho_w \) and \( \mu_w \) are density and dynamic viscosity of water respectively. \( P_c \) and \( P_a \) represent pressure at cathode and anode side of cell. Water transport in order of electro-osmotic drag is proportional to current density and is given by eq.13 [1]:

\[ n_{ed} = n_{ed0} \frac{I}{F} \]  (13)

The proportionality constant \( n_{ed0} \) depends on pressure, temperature and current density. Medina and Santarelli [15] gives a linear regression model for estimation of electro-osmotic drag coefficient (eq.14):

\[ n_{ed0} = 0.0025P - 1.6078 + 0.0197T - 2.7592 \]  (14)

2-4-SOLVING GOVERNING EQUATIONS

In order to solve the set of above nonlinear partial differential equations, at first they are discretized using finite volume method with upwind differencing scheme [17]. The obtaining nonlinear algebraic equation set, implicitly solved by using Newton linearization methods [18]. Although the implicit approach requires more computational effort at each time step than explicit approach, has the advantage of good convergency in order of independency of mesh and time step size. As a result, the one can select a fewer mesh nodes and larger time step which could lead to less computational effort to simulate whole a system [19].

2-5-INITIAL AND BOUNDARY CONDITION

Fig.2 shows the boundary conditions used for electrolyzer modeling. Inlet velocity can be obtained using mass flow rate as well as outlet pressure from vessel pressure. For void fraction, a special care must be done. Despite purity of input water a small non zero (say 0.001) is assigned to void fraction to avoid zero gas pressure. Initial conditions could be specified from a homogenous distribution of boundary conditions.

Validation of the proposed model, is done against Kim et. al. [1] model. Table.1 is summarized the data used in simulation.

Table.1: Parameters are used in validation process [1]

| Cell dimensions | Length: 0.3 m, Width: 0.105 m, Area: 0.0314 m², Number of cells: 120, Channel height: \( h_{ch} = 0.003 \) m, Electrode height: \( h_e = 0.0005 \) m, Membrane height: \( h_m = 0.0002 \) m | Constants | Electric resistance: \( r_e = 0.035 \) m\( \Omega \) | Degree of membrane humidification: \( \lambda_m = 25 \) |
Anode exchange current density: $i_{a0} = 10^{-6}$ A/m$^2$

Cathode exchange current density: $i_{c0} = 10$ A/m$^2$

Water diffusion coefficient: $D_w = 1.28 \times 10^{-10}$ m$^2$/s

Darcy’s constant: $K = 1.58 \times 10^{-18}$ m$^2$

Nominal operating condition:
- Current density: $i_{ave} = 10000$ A/m$^2$
- Pressure at the cathode: $P_c = 100$ bar
- Pressure at the anode: $P_a = 2$ bar
- Inlet water flow rate: $Q_{in} = 100$ l/min
- Inlet water temperature: $T_{in} = 55^\circ$C

Fig.3 compares performance curve of Kim et. al. and the proposed model which shows good agreement between two models.

3-SOLAR PANEL MODELING

In order to have the sufficient electricity for the electrolysis, three identical PV panel with the area on 0.9 m$^2$ are considered in series and four in parallel.

A primary electric model of a PV cell contains a current source and a diode (see Fig.4). Applying basic circuit laws gives the cell terminal voltage as:

$$V = f(I) = I L - I_D$$

(18)

Here, the light current $I_L$ depends on the solar irradiance $G$ and the cell temperature $T_c$, and is calculated according to design reference conditions:

$$I_L = \left( \frac{G}{G_{ref}} \right) \left( I_{L,ref} + k_T(T_{cell} - T_{ref}) \right)$$

(19)

where the values of $G_{ref}$, $I_{L,ref}$, $k_T$, and $T_{ref}$ are given by manufacturers. The cell temperature is a function of wind speed, solar irradiance and ambient temperature, and can be determined (in °C) with the following correlation:

$$T_{cell} = 0.9457G + 0.0286 - 1.5268V_{wind} + 4.3$$

which was developed by Chenni et al. [20] using experimental data from six solar cell technologies. The researchers state that the dependency of the cell temperature on ambient temperature, solar irradiance and wind speed are fairly independent of location.

Chenni et al. [22] present an implicit expression to calculate the maximum current of the PV cell:

$$I_{mp} = \frac{G}{G_{ref}} \frac{I_{L,ref} + k_T(T_{cell} - T_{ref})}{1 + k_T(T_{cell} - T_{ref})}$$

(21)

This expression can be solved using the Newton-Raphson method. At the maximum power point, the first derivation of power with respect to voltage is zero. Rearranging the consequent equations results in an explicit expression for the maximum voltage as a function of the maximum terminal current:

$$V_{mp} = \frac{G}{G_{ref}} \frac{I_{L,ref} + k_T(T_{cell} - T_{ref})}{1 + k_T(T_{cell} - T_{ref})} - I_{mp} R_S$$

(22)
The maximum current and voltage occurs is called the maximum power point:

$$P_{\text{mp}} = I_{\text{mp}} V_{\text{mp}}$$  \hspace{1cm} (23)

4-RESULTS AND DISCUSSION

Fig. 5 shows the power generated by solar panels during a year in Tehran. As it can be expected, solar power generation dramatically increases in hot and long days. The Voltage of this solar system is set to be 12 V. On the other hand, a 6 cells electrolyzer with cell specifications on Table. 1 (except nominal operating is selected to converting this power into hydrogen. The output pressure of gas products is set to be 1 bar and mass flow rate 2.5 l/min is determined. Fig. 6 and Fig. 7 represent current density and voltage profile of a single cell during a year. It is worth to mention that the voltage of each cell could not violet the upper limit which 2 V. As can be seen in Fig. 6 sometimes in the middle year the voltage of each cell reaches the upper limit which leads to a limitation on the maximum of current density (fig. 7). It can be shown that the electrolyzer power consumption would be different (usually less) from available solar power. This means some of solar power would be lost without any useful usage (Fig. 8). As it is illustrated in Fig. 8, the lost power in time is not so much (less than 100 W). Fig. 8 shows the profile of hydrogen mass flow rate produced from this solar hydrogen production system. To pressurizing produced hydrogen two strategies are existed. First, low pressure hydrogen production and compressing it using a compressor to create high pressure hydrogen. The second one is high pressure electrolysis which produces high pressure hydrogen up to 130 bar. If more pressure is needed it can be compressed using a compressor. In this paper investigate high pressure electrolysis with hydrogen vessel pressure equals to 100 bar. The target pressure of final product is set to 350 bar to be useful for some vehicle applications. Specific compressor work can be calculated using eq. 24:

$$W = C_p T_0 \left( \frac{P_2}{P_1} \right)^{\frac{k-1}{k}} \frac{P_2}{\eta_c}$$  \hspace{1cm} (24)

Total efficiency of hydrogen production system is calculated using eq. 25:

$$\eta_{\text{sys}} = \frac{m_{\text{H}_2} V_{\text{H}_2}}{P}$$  \hspace{1cm} (25)

Where HHV represents high heat value of hydrogen, while $m_{\text{H}_2}$ and $P$ are total hydrogen production and total solar power generation respectively.

Fig. 5: Solar Power generation profile in Tehran
In Fig. 10 accumulated hydrogen production is presented. As expected, the hydrogen production for high pressure electrolysis is decreased. However, the specific compressor work to produce high pressure hydrogen would be decreased. The average specific work and efficiency of two strategies are summarized in the Table 2 by the assumption of 50% efficiency for hydrogen compressor [7]. As it can be seen in the Table 2 although the work of compressing the hydrogen is lower in the second strategy, the system efficiency is significantly lower than first strategy. Fig. 11 reveals the cause of this phenomena. In order to high pressure electrolysis the Nernst voltage of cell would be increased. As a result at the specific cell voltage, the maximum current density would be lower which leads to more losing power when the cell reached the upper voltage limit (2V).
CONCLUSIONS
In this paper, a one dimensional dynamic model for the PEM electrolyzer was proposed. The proposed model is suitable for system design and analysis thank to capability of selecting large time step and lower mesh nodes. Using this model the performance of a solar hydrogen production system was evaluated. Simulation of PV panel is carried out using TRNSYS software and the weather data of Tehran. The results shows that for an integrated system, some of solar power could not be used by electrolyzer so it is lost. Also, high pressure electrolysis is not always an appropriate and efficient choice. In fact, in the system level simulation, all components and their performance must be carefully considered for improving system efficiency.

KEYWORDS
Solar cell, PEM, electrolyzer, Hydrogen production, Dynamic modeling,
REFERENCES


16. BERTOLA, VOLFANGO. MODELLING AND EXPERIMENTATION IN TWO-


