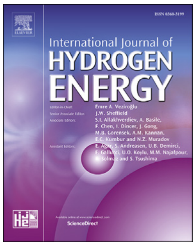
INTERNATIONAL JOURNAL OF HYDROGEN ENERGY XXX (2017) 1–6

Available online at www.sciencedirect.com

ScienceDirect

journal homepage: www.elsevier.com/locate/he



Multiphysics simulation of pulsed cold plasma arc rotation for enhanced hydrogen harvesting

Minxiang Wu[*], *Jose Pacheco*, *Eva Cosoroaba*, *Babak Fahimi*

The University of Texas at Dallas, 800 West Campbell Rd., EC33, ROOM 3.320, Richardson, TX 75080, USA

ARTICLE INFO

Article history:
Received 27 July 2017
Received in revised form
8 September 2017
Accepted 24 September 2017
Available online xxx

Keywords:
Arc
Cold plasma
Magnetic field
Multiphysics

ABSTRACT

Pulsed cold plasma reforming is a novel method to harvest hydrogen from hydrocarbons. The harvested hydrogen can feed a fuel cell for distributed generation of electricity in a stationary or mobile platform. The cold plasma arc is generated by a pulsating high voltage waveform. The arc rotates in the magnetic field caused by a ring permanent magnet, thus increasing the collision area between the arc and the fuel. Due to the difficulties of measurement of plasma properties such as ion and electron temperature without disturbing the plasma, multiphysics simulation is a key step in the design of electrodes, thereby increasing the hydrogen harvest rate in the syngas. In this paper, a 3D multiphysics simulation including fluid dynamics, thermal response, and electromagnetic fields has been carried out to assist in selection of the permanent magnet. Experiments were carried out to verify the simulation results. The 3D multiphysics simulation is demonstrated to be an effective tool to assist in the design of the reformer. The hydrogen harvest rate has been improved from 58.7% to 67.8% with the introduction of the magnet.

Introduction

Hydrogen, as a clean energy carrier, reduces carbon emissions. With the fast development of fuel cell vehicles, the demand for hydrogen is increasing [1]. The mainstream production of hydrogen is through steam reforming, requiring high temperature and large scale facilities [2]. The distribution is through high pressure gas cylinders. The installation of hydrogen cylinders in households without professional handling can be dangerous. Compared to steam reforming, the pulsed cold plasma reforming method is a promising way to generate hydrogen in small scale stationary and mobile platforms [3,4]. Plasma assisted reforming technologies [5–17], including dielectric barrier discharge [5], arc discharge [6–8], corona discharge [9], and microwave plasma [10,11], have been used to generate hydrogen rich output. Different fuel for hydrogen production with cold plasma include methane [12], methanol [13–15], ethanol [16], and diesel [17]. Methanol has high energy density and high hydrogen to carbon ratio compared to other liquid fuels [4]. Moreover, the distribution of methanol is safer and cheaper than that of hydrogen, which makes methanol an attractive fuel. The pulsed cold plasma reforming does not need pre-heating of the reactants to thousands of degrees. The pulsed cold plasma reforming method uses high voltage to form arcing, creating electrons and ions in the cold plasma chambers and in the presence of hydrogen rich fuels. The accelerated electrons and ions break the chemical bond in the methanol and water mixture. Subsequently the radicals recombine to form hydrogen. Since the chemical bond only need to be broken once, the time needed for arcing is relatively small compared

---

[*] *Corresponding author.*
E-mail address: mxw130030@utdallas.edu (M. Wu).

https://doi.org/10.1016/j.ijhydene.2017.09.143
0360-3199/© 2017 Hydrogen Energy Publications LLC. Published by Elsevier Ltd. All rights reserved.

Please cite this article in press as: Wu M, et al., Multiphysics simulation of pulsed cold plasma arc rotation for enhanced hydrogen harvesting, International Journal of Hydrogen Energy (2017), https://doi.org/10.1016/j.ijhydene.2017.09.143

to that of recombination. By using pulsed cold plasma instead of maintaining the continuous arcing, electric energy for the arc can be saved and the efficiency for hydrogen production is increased.

To design the cold plasma reformer with better efficiency, multiphysics simulation including fluid dynamics, thermal, and electromagnetics analysis is proposed in this paper. Since the density of the electrons and ions is high as compared to normal plasma working conditions and the arc column is very small, the measurement of electron temperature using Langmuir probes without disturbing the arc is extremely difficult. With the help of the multiphysics simulation, the temperature of the arc can be estimated, which is crucial for the system design. Researchers performed significant modeling work for the arc plasma torches. They developed models for both local thermal equilibrium (LTE) and non-equilibrium models (NLTE) to estimate the plasma temperatures, the voltage drop, current, and arc length [18–20]. Furthermore, the flow rate of the reactants can be estimated, to make sure that the arc only strikes the molecules once. The multiphysics simulation is the foundation for the optimal design process of the system, adding the determination of variables such as the electrode shapes, flow rate, voltage duty cycle, and mixture concentration.

In this paper, a 3D multiphysics simulation of the pulsed cold plasma reforming has been carried out to assist in designing the reformer. Experiment have also been conducted to validate the multiphysics simulation and to illustrate that the hydrogen harvest rate has been improved.

Modeling of pulsed cold plasma

When the arc occurs, the reaction chamber is at atmospheric pressure, which is relatively high pressure compared to the plasma formed in a partially vacuumed chamber. The number of ions and electrons which exists in the plasma is extremely large, hence the arc column between the cathode and the anode is assumed to be in local thermodynamic equilibrium (LTE). This means the temperature of the ions is the same as that of the electrons. The plasma in the arc column can be assumed to be a conducting fluid. To describe this conducting fluid, the equations of mass, momentum, and energy conservation are included.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0 \qquad (1)$$

where ρ, υ are electron density and electron velocity.

$$\frac{\partial (\rho \boldsymbol{v})}{\partial t} + \boldsymbol{v} \cdot \nabla (\rho \boldsymbol{v}) = -\nabla P + \nabla \cdot \boldsymbol{\tau} + \boldsymbol{j} \times \mathbf{B} + \rho \boldsymbol{g} \qquad (2)$$

where P, τ, j, B are electron pressure, viscous stress tensor, current density and magnetic flux density.

$$\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho h \boldsymbol{v}) = \nabla \cdot \frac{k}{C_P} \nabla h + \boldsymbol{j} \cdot \mathbf{E} - S_{rad} \qquad (3)$$

where h, k, C_p, E, S_{rad} are enthalpy, thermal conductivity, specific heat, electric field strength, and the radiation losses.

Simulation of cold plasma

Plasma arc formation

When a high voltage pulse is applied across the electrodes, the electrons and ions in the electrodes are accelerated. As the voltages increases, the electrons gain energy and finally break through the airgap. In the process of moving to the other electrode, the electrons and the ions collide with other neutral molecules in the chamber, creating more electrons and ions. Therefore, a pathway of the arc is formed. Arc occurs at the airgap between the top electrode and the bottom electrode. The simulation setup is shown in Fig. 1. The gas mixture is methanol and water (steam) with a mole ratio of 1:1. The length of the airgap is 8 mm. The inner diameter of the electrode is 3.86 mm whereas the outer diameter of the electrode is 6.35 mm. Electrode material in the simulation is stainless steel, same as in the experiment. The temperature of the electrons and ions is the main characteristic of the plasma. As the temperature of the electrons increases, the density of electrons increases and the resistance of the arc reduces.

A simulation has been carried out using COMSOL Multiphysics to simulate the arc formation and the electron temperature. The temperature boundary condition of the inlet is 100 °C. The temperature boundary condition of the outlet and the quartz is 25 °C. The pressure in the inlet and the outlet is 1 atm. In this simulation, the conductivity of plasma depends on temperature. Furthermore, the temperature of the plasma is related to the current density. The coupled simulation of current and thermal provides the current density and temperature distribution. Magnetic field is induced by the current according to Ampere's law. The arc between the electrodes occurs at 10.6 μs after the ramp voltage up to 8 kV is applied. The temperature distribution is shown in Fig. 2, which represents as a perpendicular slice. Fig. 3 shows horizontal slices:

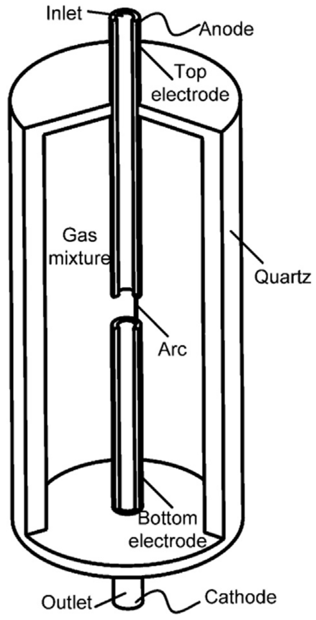


Fig. 1 – The simulation setup.

Please cite this article in press as: Wu M, et al., Multiphysics simulation of pulsed cold plasma arc rotation for enhanced hydrogen harvesting, International Journal of Hydrogen Energy (2017), https://doi.org/10.1016/j.ijhydene.2017.09.143