CHEMICAL ENGINEERING RESEARCH AND DESIGN 90 (2012) 1871–1882

Contents lists available at SciVerse ScienceDirect

Chemical Engineering Research and Design

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

Dynamic modelling and sensitivity analysis of a tubular SOFC fuelled with NH_3 as a possible replacement for H_2

S.A. Hajimolana, M.A. Hussain, W.M.A. Wan Daud, M.H. Chakrabarti*

Department of Chemical Engineering, University of Malaya, 50603 Kuala Lumpur, Malaysia

ABSTRACT

A dynamic model of an ammonia fed-tubular solid oxide fuel cell (NH_3-SOFC) is developed and presented. The model accounts for diffusion, inherent impedance, transport (heat and mass transfer), electrochemical reactions, activation and concentration polarizations of electrodes and the ammonia decomposition reaction. Sensitivity analyses are conducted upon the effects of design parameters on the fuel cell performance. Dynamic output voltage, fuel-cell-tube temperature and efficiency responses to step changes in the inlet fuel flow pressure with different values of design parameters are discussed. It is found that among the studied parameters, the inner cell tube diameter has the strongest effect on fuel cell efficiency. On the other hand, the influence of cathodic porosity on fuel cell performance and transient response is higher than that of the anodic porosity. The transient response with different sizes of micro and macro-structures is studied and it is observed that changing the fuel cell length has the most effect. Also NH_3-SOFC is compared with H_2-SOFC and it is found that the performance of the former is close to that of the latter thus signifying that ammonia is a suitable fuel for substituting in place of hydrogen.

Keywords: Ammonia fuel; Hydrogen fuel; Thermal efficiency; Transient response; Ammonia decomposition

1. Introduction

Solid oxide fuel cells (SOFCs) can generate electricity at high fuel efficiencies (typically in the range of 45–60%) (Skyllas-Kazacos et al., 2011; Chakrabarti and Roberts, 2008). Such high efficiencies are a significant competitive advantage over other technologies. In addition, SOFCs offer high power density, low cost, scalability, fuel flexibility and superior durability.

One of the most glowing advantages of SOFCs over other types of fuel cells, such as proton exchange membrane fuel cell (Srinivasarao et al., 2011; Tashima et al., 2011), is that a variety of fuels can be applied (Sadhukhan et al., 2010; Hajimolana et al., 2011; Bavarian and Sorosuh, 2012). Although hydrogen (H_2) is usually the preferred fuel of choice as high power densities can be obtained, effective and economical production and storage of hydrogen as well as its refuelling infrastructure are still facing major challenges (Ma et al., 2006). It is therefore important to use alternative fuels in SOFCs such as bio fuels and ammonia. Ammonia is a good hydrogen carrier and may be an excellent substitute for hydrogen and hydrocarbons due to several reasons. Firstly, the price of ammonia is as competitive as that of hydrocarbons. Secondly, ammonia can be easily liquefied under about 10 atm at ambient temperatures or at −33 °C under atmospheric pressure and the volumetric energy density of liquefied ammonia is about 9×10^6 kJ/m^3, which is higher than that of liquid hydrogen, making it useful for transportation and storage. Thirdly, ammonia is less flammable compared with the other fuels and the leakage of ammonia can easily be detected by the human nose under 1 ppm. Fourthly and most importantly, there are no concerns about anodic coking, since all the by-products of the electrode reaction are gaseous (Ma et al., 2006). All of the above imply that ammonia could be an ideal candidate as a liquid fuel for SOFCs, at least at the present stage when the coking problem of hydrocarbon fuels has not yet been resolved.

Although much experimental work has been done on ammonia-fuelled solid oxide fuel cells (NH_3-SOFCs) (Ma et al., 2006; Pelletier et al., 2005; Wojcik et al., 2003; Limin and Yang, 2008; Fournier et al., 2006; Meng et al., 2007; Ma et al., 2007; Maffei et al., 2005, 2006, 2008), only few research studies are available on mathematical modelling of the NH_3-SOFC (Ni et al., 2008a,b,c; Ni, 2011; Siamak and Hamdullahpur, 2010).

* Corresponding author. Tel.: +60 3 79675206.
E-mail addresses: mohd_azlan@um.edu.my, yashar_molana1@yahoo.com (M.A. Hussain).
Received 10 June 2011; Received in revised form 28 January 2012; Accepted 5 March 2012
0263-8762/$ – see front matter
doi:10.1016/j.cherd.2012.03.004