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SIMULATION AND OPTIMIZATION OF A BUTANE AUTOTHERMAL REFORMER FOR FUEL CELL APPLICATIONS

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Abstract. Hydrogen (H_2) production is gaining popularity among researchers for a better future environment. Hydrogen, which is known as the cleanest fuel, is also an excellent candidate to replace existing fuels. Its high flammability and energy produced with no side product make it even more popular. In this study, a steady-state model simulation is developed to describe a butane fuel processor by autothermal reforming (ATR) to provide H_2 for fuel-cell application. The objective of the study is to develop a general steady-state simulation of an H_2 production plant for fuel cell application using butane as the feedstock. The scope of the study includes stoichiometric mathematical analysis, base case steady-state simulation, base case simulation validation, the design of heat integration, carbon monoxide (CO) clean-up processes which contains water gas shift (WGS) and preferential oxidation (PrOx) reactors and plant wide optimization. The simulation has been run in Aspen HYSYS 2004.1 in steady-state mode in which optimization was done to generate more H_2 as well as CO reduction. The butane fuel processor was optimized at Oxygen-to-Carbon (O/C) ratio of 2.18 and Steam-to-Carbon (S/C) ratio of 4.6 to produce 39.2 % of H_2 and has achieved 78.1 % efficiency, while CO clean-up units was capable to reduce the CO concentration down to 10 ppm.

Key Words: Butane, Autothermal Reforming, Proton Exchange Membrane Fuel Cell, Aspen HYSYS, Simulation and Optimization

1.0 INTRODUCTION

Hydrogen as an energy carrier in proton exchange membrane fuel cell (PEMFC) offers perhaps the largest potential benefits in terms of reduced emissions of pollutants and greenhouse gases. Moreover, no side products are involved in the electrochemical conversions of H_2 with zero emission of hazardous species, for instance volatile organic compound (VOCs), nitrogen oxides (NO_x) and carbon oxides (CO) [1]. When it is used as fuel, it will only produce water. It is such a good option as a fuel because H_2 is colourless, odourless and extremely flammable and also the smallest and simplest member of the family of chemical elements compared with other fuel such as hydrocarbons, alcohols, or coals [2].

However, it is difficult to store and handle hydrogen directly as a kind of on-board fuel. For practical fuel cell systems hydrogen gas has to be generated from locally available fuels, most commonly hydrocarbons. The objective of this study is to simulate and optimize the on-board hydrogen production for fuel cell vehicle from hydrocarbon feedstock. This study is important since the on-board conversion of hydrocarbon feedstock

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