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## Optimization of Jet-A fuel reforming for aerospace applications

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#### Abstract

This paper focuses on the optimization of Jet-A fuel reforming for use with solid-oxide fuel cells in aerospace applications. Because of the specialized operating conditions and reforming requirements, a broad range of reforming inlet conditions need to be considered. Both equilibrium calculations for reforming of a Jet-A surrogate and zero-dimensional modeling with detailed chemistry for reforming of a kerosene surrogate are performed over a wide range of conditions with varying inlet temperature, operating pressure, steam-to-carbon ratio, and oxygen-to-carbon ratio. While equilibrium calculations provide some insight into the efficiency of the final reformer, the kinetics modeling can account for the finite residence time of the gas within the reformer. Calculations using finite-rate gas-phase chemistry indicate that the most efficient mode of reforming is achieved using a short-contact partial oxidation reactor operating with minimal water addition. Certain factors to consider for the development of a future catalytic reformer, such as local hot-spots and coke deposition on the catalyst, are also discussed. © 2006 International Association for Hydrogen Energy. Published by Elsevier Ltd. All rights reserved.

Keywords: Reforming; Jet fuel; Syngas

### 1. Introduction

The merging of fuel cell (FC) power technology with aerospace applications holds the key to the creation of less-polluting and more efficient aircraft. Theoretically the electro-chemical process that takes place within the fuel cell is significantly more efficient than IC engines in converting the fuel chemical energy into electrical or mechanical energy. Fuel cells can also be used to store electrochemical energy, with much larger energy density ( $\sim 2500$  Wh/kg for reformed methanol [1]) than conventional batteries ( $\sim 150$  Wh/kg for lithium battery). Their lack of vibration, ease of scalability, and reduced emissions make them an attractive power plant for future aircraft.

One type of fuel cell, the solid-oxide fuel cell (SOFC) [2–4], stands out as the prime candidate for future aerospace systems. This ceramic-based fuel cell tolerates fuel impurities better than other FCs. Its high operational temperature (900–1300 K [2]) allows CO to be used as a fuel, eliminating the need to convert CO to CO<sub>2</sub>. The high-temperature exhaust also allows increased efficiency by utilizing a hybrid SOFC/gas turbine engine to extract work out of the exhaust, and also provides a thermal feedback mechanism that can be utilized to reduce the losses involved in fuel reforming [5]. A sample SOFC–hybrid power plant for aerospace applications, capable of providing 200 kW of electrical power has previously been proposed by Freeh et al. [6].

FC power plants require the use of hydrogen gas as the primary fuel. Hydrogen is not readily available on earth, and must be either produced from fossil fuels or from water by adding large quantities of energy. The conversion of hydrocarbon fuels into hydrogen-rich gas

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(or the so-called "syngas"), known as reforming [3,7–9], can be performed either at centralized facilities or onsite, using specially designed fuel reformers. The direct use of hydrogen fuel is hampered by the difficulties involved in its storage (high-pressure gas or cryogenic system), and the large volumes required (due to its low density). Liquid hydrocarbon fuels, including aviation fuels, provide a much larger amount of chemical energy per unit volume than hydrogen. The use of common fuels, such as gasoline, diesel, and jet-fuel, also eliminates the need to provide specialized fueling infrastructure. On-site reforming, therefore, offers the best alternative for applications where weight is a concern. In terms of available hydrocarbon fuels, Jet-A fuel [10] has a low concentration of impurities and is widely used in the aerospace industry, making it an ideal fuel to use for aeronautical fuel cells.

The present study aims to identify the optimal conditions for the on-site reforming of Jet-A fuel for aerospace applications. The study focuses on the reforming of fuels with hydrogen-to-carbon ratios of 1.92-2.06, making it relevant to kerosene-based fuels (such as Jet-A). The predicted reformer output is optimized for the current requirements, including minimization of the reformer volume and reactant weight. When taking these considerations into account, several previously-unexplored topics, such as the finite residence time and water weight, become important. Fuel reforming can be performed either in the gas-phase (non-selective), or in the presence of a catalyst (selective). The present work addresses only the gas-phase chemical process, or non-selective reforming. Although the catalyst will accelerate the reforming process by enhancing the overall reactivity, the final equilibrium temperatures and product concentrations for a given initial mixture will be identical, regardless of the reaction mechanism. In this manner, the current gas-phase results are still relevant to the catalytic process, and can also shed light on the operating conditions of selective reforming, especially the critical issues related to local hot-spots and coke deposition on the catalyst.

In the following, we will first briefly highlight the scientific background regarding fuel reforming. Four key variables, which control the reformer output temperature, mixture composition, and overall efficiency, are considered herein. They include inlet temperature, operating pressure, steam-to-carbon ratio (S/C), and oxygen-to-carbon ratio ( $O_2/C$ ). It is noted that in reality, other factors will also play a role, such as: residence time, catalyst reactivity, reaction pathway, peak temperature, and coke deposition. Numerical models used to asses the reforming efficiency and limitations

for a wide range of operating conditions are described next. Subsequently, the performance of the reformer, as predicted using equilibrium calculations, is presented. These equilibrium calculations will give the maximum achievable reformer output, assuming infinite residence time. Finally, results obtained using a time-dependent model, with detailed chemical kinetics, are discussed; which will provide further insight into the limitations of a real-world reformer.

#### 2. Fuel reforming

The goal of fuel reforming for SOFCs is to maximize the output of  $H_2$  and CO per fuel molecule. This must be done while avoiding complete oxidation of the gas into CO<sub>2</sub> and water. Reforming of hydrocarbons (HCs) is normally performed using either the endothermic steam reforming (SR) reaction [cf. [3,11]]:

$$C_m H_n + m H_2 O \rightarrow m CO + (m + n/2) H_2, \qquad (1)$$

or the exothermic partial oxidation (PO) reaction in a fuel rich system [cf. [3,12,13]]:

$$C_m H_n + (m/2)O_2 \to mCO + (n/2)H_2.$$
 (2)

We shall refer to reaction (2) as *direct* PO of the fuel. The use of oxygen in PO of the reactant feed may also lead to the highly exothermic total oxidation reaction [12,13]:

$$C_m H_n + (m + n/4)O_2 \rightarrow mCO_2 + (n/2)H_2O.$$
 (3)

In the presence of water, the reforming reactions (1) and (2) will normally be followed by the water-gas shift (WGS) reaction [cf. [3,11]] which further converts CO into CO<sub>2</sub> and produces additional  $H_2$ :

$$\mathrm{CO} + \mathrm{H}_2\mathrm{O} \to \mathrm{CO}_2 + \mathrm{H}_2. \tag{4}$$

It is possible to combine several reforming steps by having the total oxidation step, reaction (3), followed by reactions (1) and (4). In this manner, the water produced by combustion is used for steam reforming of the leftover fuel. This type of reforming processes is sometimes referred to as the *indirect* PO reforming process. There is still much debate over which pathway, indirect or direct, dominates the partial oxidation of the fuel [12,13]. Although it is possible to predict the final products of reforming using an equilibrium calculation, such analysis will not reveal which reactions dominate. This information, however, may be of extreme importance in order to avoid local hot-spots, carbon deposition, or extremely slow reaction pathways. Download English Version:

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