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Review Article

Effect of Oxygen Concentration on Distributed Flame Regime

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Abstract

This work investigated the effect of oxygen concentrations in the reactor on the partial oxidation of JP8 under the distributed reaction condition. Reforming efficiency as high as 74% was achieved; syngas composition consisted of 20.7 to 22.3% hydrogen and 20.2 to 21.5% carbon monoxide. Reformate product distribution and quality was found to depend on the reactor oxygen concentrations and to a lesser extent on flame regime. Addition of oxygen enhanced the extent of reforming reactions, to promote increased conversion and reforming efficiency.

Keywords: Fuel reforming, Syngas, Distributed flame regime, JP8 fuel reforming, Reactor oxygen concentration, Reformer efficiency

1 Introduction

Jet Propellant 8 (JP8) is a particularly challenging fuel to reform in conventional catalytic reformers [1]. JP8 has a maximum allowable sulfur content of 3,000 ppm, which will deactivate most reforming catalysts [1]. Additionally, the high aromatic and carbon content of JP8 promotes the coking of the reforming catalyst. Common reforming catalysts are costly, as they generally contain platinum, rhodium, and other noble metals. A non-catalytic approach avoids issues arising from incompatibility of the fuel and reforming catalysts, but is often less efficient and generates high yields of soot. Reformers typically operate with limited mixing, as they operate under laminar flow conditions [2]–[12].

Reforming in the premixed turbulent distributed reaction regime can avoid soot formation and generate higher reforming efficiencies. This approach has achieved reforming efficiency as high as 80% under wet partial oxidation conditions. Previous work [2] investigating wet partial oxidation conditions, placed an emphasis on developing an understanding of steam reforming effect under distributed reaction regime. However, the results showed that greater emphasis should be placed on understanding the effect of partial oxidation reactions on the reformate composition.

Oxygen fostered greater conversion through artial oxidation reaction. In addition, the more distributed condition (lower O/C ratios) produced less combustion products, minimizing the reactions caused by the entrained products. Reactor oxygen concentrations were varied to reveal the impact on the thermochemical behavior and reformate product distribution. Flame operational regime was calculated through numerical methods.

2 Experimental Facility Design

Experimental facility design was similar to the

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experimental setup used in Scenna and Gupta [6]. Oxygen-to-carbon ratios were used to control the chemical time and length scales, while injection temperature was maintained at 375°C. The reactor was operated at a thermal load of 4.4 to 5.1 kWth. Reactor residence time remained near constant, only varying between 820 to 830 ms. Air and fuel feeds were independently heated, then mixed prior to injection. Fuel was vaporized at 300°C, which was high enough to allow complete vaporization, while simultaneously low enough to prevent carbon formation [8]. The reactor consisted of an external steel pressure vessel, which was lined with high-purity alumina insulation. The alumina liner served to both insulate and shield the external pressure vessel from the reducing environment. Alumina liner was divided into four segments to relieve thermal stresses and extend the reactor life. The steel pressure vessel was inserted into a tube furnace and maintained at 800ºC. By reducing the temperature gradient, near adiabatic conditions were achieved.

Jet Propellant 8 (JP8) used in this work had 14.4% hydrogen concentration by mass and a heating value of 43.6 MJ/kg. Chemical analysis by the manufacturer indicated sulfur concentrations of 30 ppm. Reactor temperatures were maintained under 1,200°C to foster structural rigidity of the exhaust or thermocouples.

3 Reactor Operating Condition

At lower reactor temperatures, the oxygen-to-carbon ratio (O/C) had a significant impact on reformer performance and reaction regime [3]. This work revealed peak performance at an O/C ratio of 1.10; therefore, O/C ratios between 1.04 and 1.20 were explored. The O/C ratio was adjusted to explore the impact on the distributed reaction regime at higher temperature reactors (900–1,000°C). Significant soot formation occurred under Flamelet in eddies regime and resulted in blockage of exhaust line. The reactor was only operated within the distributed reaction regime to enhance the reactor operational time. Reactants were injected at a fixed injection temperature of 375°C. In addition, reactor temperatures were restricted to 1,200°C to mitigate any undue maintenance and promote operational times of the reactor and thermocouples.

4 Premixed Turbulent Flame Regime

Flame regime was determined through numerical calculations. Transport properties were calculated using the Fluent commercial CFD code. Chemical properties were determined using the numerical solver Chemkin [10] and a reduced kinetic mechanism consisting of 121 species and 2,673 reactions [11]. JP8 was represented using a surrogate proposed by Viola, which has previously been verified to predict flame speed [12].

Under all conditions evaluated (preheats of 375°C and O/C = 1.04–1.20), the reactor operated within the distributed reaction regime. An increase in oxygen content fostered a more rapid chemical reaction, which increased flame speed from 9.99 cm/sec to 13.12 cm/sec and decreased laminar flame thickness from 0.41 cm to 0.35 cm. Integral length scale and turbulent velocity remained unaffected by an increase in O/C ratio, both remaining constant at 1.88 mm and 1.28 m/s, respectively.

4.1 *Reformate composition*

Reformate chemical composition was strongly influenced by the availability of oxygen and to a lesser extent the flame regime. Syngas composition consisted of 20.7–22.3% hydrogen and 20.2–21.5% carbon monoxide, see Figures 1 and 2. Carbon dioxide was detected at concentrations of 2.35–2.85%.

Up to an O/C ratio of 1.10, an increase in oxygen content promoted higher concentrations of hydrogen. Under regimes of low conversion, the reactor generated low yields of syngas. Under this condition, an increase in oxygen content was more likely to oxidize the unconverted hydrocarbons than the limited syngas produced. At O/C ratios greater than 1.10, a reduction in hydrogen concentrations was noted. As conversion increased at higher O/C ratios, the reactor generated higher yields of syngas and lower yields of unconverted hydrocarbons. Under this condition, oxygen became more likely to oxidize the more abundant syngas than the remaining hydrocarbons. This is supported by a small increase in reactor temperature.

In the low temperature reactor detailed in Scenna and Gupta [3], air preheats of 450°C resulted in peak hydrogen formation occurring at a similar O/C ratio (O/C = 1.10). However, hydrogen concentrations were almost twice what was reported at lower operating temperatures. Higher reactor temperatures promoted

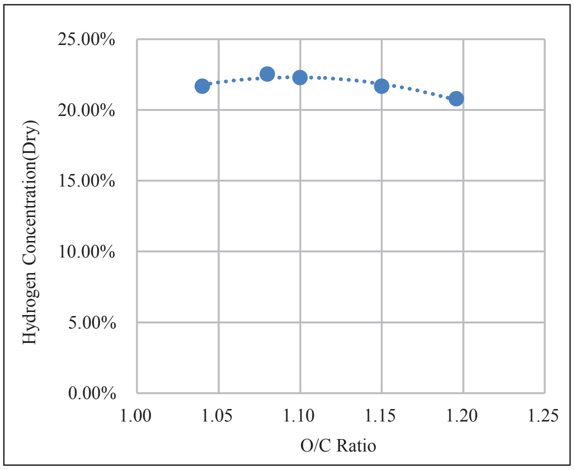

Figure 1: Hydrogen concentrations at O/C = 1.04 to 1.20.

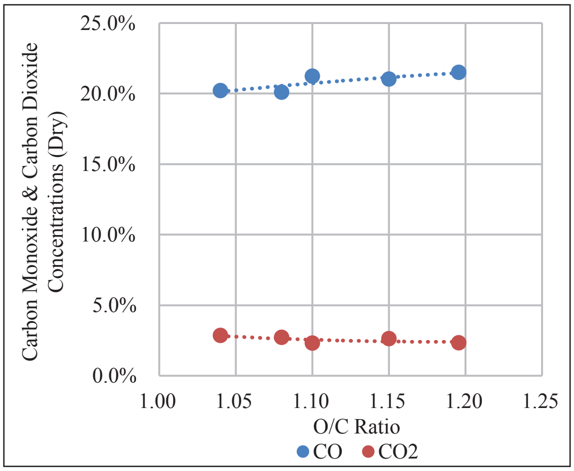

Figure 2: Carbon monoxide and carbon dioxide concentrations at O/C = 1.04 to 1.20.

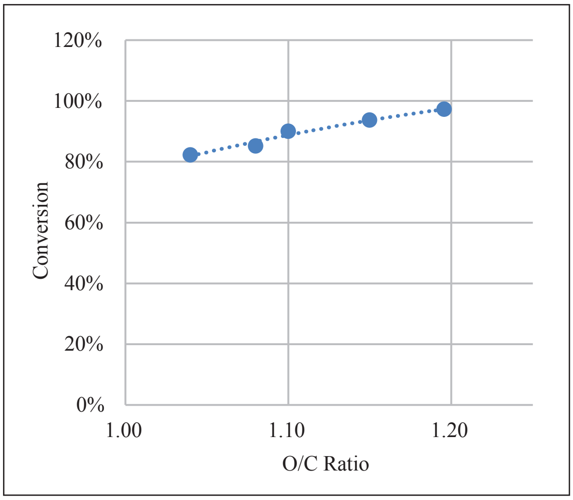

Figure 3: Fuel conversion at O/C = 1.04 to 1.20.

the dissociation, steam reforming, and dry reforming of hydrocarbons, which enhanced conversion.

In comparison, when operating at lower reactor temperatures (700–800°C) as detailed in Scenna and Gupta [3], preheats of 450ºC generated a wide range of hydrocarbons, ranging from 5% methane to 0.18% hexane. The lower reactor temperatures suppressed the dissociation, steam reforming, and dry reforming of hydrocarbons. This in turn caused the excess oxygen to oxidize the syngas (carbon monoxide and hydrogen), resulting in higher water and carbon dioxide yields. Operating at higher reactor temperatures (900–1,100°C) promoted the dissociation of lower series of hydrocarbons (CH_4, C_2H_2, C_2H_4), which enhanced syngas yields and fuel conversion.

Reforming efficiency (η_{reff}) is a measure of the usable energy obtained after the reforming process. Typically, it is defined as a ratio of the lower heating value of the hydrogen and carbon monoxide to the lower heating value of the fuel. Under ideal conditions (reformate only consists of hydrogen and carbon monoxide) a maximum reforming efficiency of 85% was achieved. Reforming efficiency is presented in Equation (1). Note that reforming efficiency is presented only for proton exchange membrane fuel cells, as only low concentrations of hydrocarbons were produced and will not impact the reformate quality.

$$\eta_{reff} = \frac{LHV\ (H_2 + CO)}{LHV\ (Fuel)} \tag{1}$$

The availability of oxygen limited the extent of the reforming reactions. Increasing oxygen content fostered a more rapid chemical reaction, which shortened chemical time and length scales, resulting in less distributed conditions. In previous works [2], [6], this would have resulted in poorer reformate quality. However, the negative effects of the reactor becoming less distributed were offset by the increased availability of oxygen. As the reactions were limited by the availability of oxygen, the addition of oxygen enhanced the extent of reforming reactions, promoting increased conversion (Figure 3) and reforming efficiency (Figure 4).

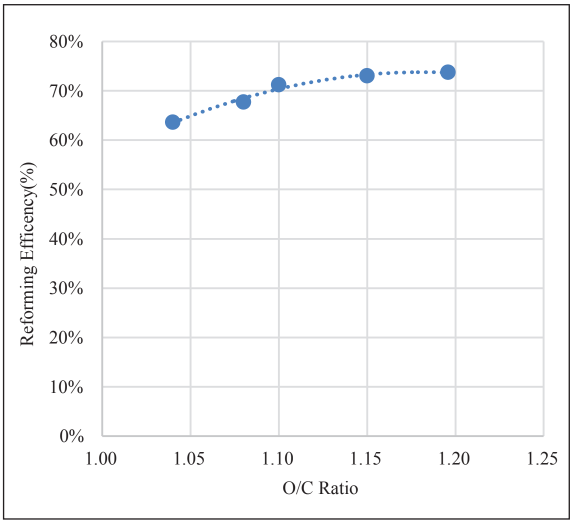

Figure 4: Reforming efficiency at O/C = 1.04 to 1.20.

5 Conclusions

Oxygen content has a pronounced effect on the distributed reaction regime and reformate yields. Increasing reactor oxygen concentrations helped greater conversion from partial oxidation reactions, directly improving reforming efficiency. Reformate composition was strongly influenced by the availability of the limiting reactant (oxygen) and to a lesser extent flame regime.

An increase in O/C ratios fostered a more rapid chemical reaction, which shortened the chemical time and length scales, resulting in a less distributed reactor. In previous works [2], [6], this would have resulted in poorer reformate quality. However, the negative effects of the reactor becoming less distributed were offset by the increased availability of oxygen. As the reactions were limited by the availability of oxygen, the addition of oxygen enhanced the extent of reforming reactions, promoting both increased conversion and reforming efficiency.

Syngas composition consisted of 20.7–22.3% hydrogen and 20.2–21.5% carbon monoxide. Low concentrations of methane and ethane were observed that ranged from 0.12 to 0.28% and 0.01%, respectively. The reformer demonstrated a reforming efficiency of 63–74% and conversion of 82–97%.

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