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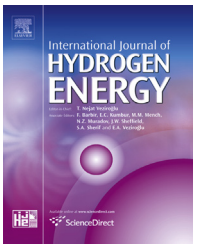

Modelling hydrogen production by the rich combustion of heavy fuel oil

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ABSTRACT

This paper reports on a modelling study of the rich combustion of heavy fuel oil in a reactor packed with an inert porous medium. Decalin is used as a model compound to represent the heavy fuel oil. A computational model is developed for the reactor, based on a two space dimensional transient heterogeneous description, and a kinetic global model for partial oxidation reforming of decalin is proposed. Also, equilibrium calculations were performed for the experimental conditions of the study. The experimental and simulation results show that heavy fuel oil is a potential fuel to produce hydrogen. It is concluded that notable characteristics of the process can be observed by simulation: the presence of an axial maximum in the production of H_2, and positive effects of the equivalence ratio and filtration velocity increase and heat losses reduction on the fuel conversion to H_2.

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Introduction

Synthesis gas, also known as syngas, is a mixture of hydrogen and carbon monoxide that is extensively used as a chemical feedstock, as well as being an important source of hydrogen. It can also be used for enrichment of traditional combustors, or as a way to produce a high quality fuel from a feed of low energy content or from carbon neutral sources (e.g. biodiesel, vegetable oil, and waste oil). Syngas can also be used to generate electricity by direct combustion, for the operation of high-temperature fuel cells (MCFC and SOFC), or in the production of value added chemicals (e.g. methanol, higher alcohols, detergents and ammonia) [1,2]. Syngas can be produced from various hydrocarbon sources, including natural gas, liquefied petroleum gas (LPG), fuel liquids, coal and biomass. The partial oxidation of liquid fuels is a promising method for hydrocarbon production, and its use in reactors containing an inert porous medium (IPM) has garnered considerable interest over the last 20 years. The use of an IPM for homogeneous gas phase reactions is known as filtrational gas combustion. During this process, the combustion reaction occurring in the porous medium can be described by one of the following steady-state regimes, which in turn depend on the propagation velocity of the thermal wave. The *low-velocity regime* (LVR) has flame propagation velocities of the order of 10^{-4} m/s, whilst the *high-velocity regime* (HVR) has a wave velocity of approximately 10 m/s. In the *sound velocity regime*

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(SVR) the wave velocity is approximately 100 m/s. As the wave velocity increases, we encounter the low-velocity detonation (LVD) at 800–1500 m/s followed by the normal detonation with losses region (ND) at 1500–2000 m/s [3].

The inert porous medium in the reactor usually consists of pellets of varying geometries that are randomly packed. Heat transfer effects are especially important in the bed, and occur by conduction and radiation between the particle surfaces, and by convection between the solid and gas [4,5]. The reactions and heat transfer mechanisms control the temperature, which may differ significantly from the adiabatic value. The reactors can be operated in either the stationary or transient mode. Steady state operation is widely practised in radiant burners and surface combustor-heaters, where the combustion zone is stabilized within the finite element of the porous matrix. Transient operation involves a travelling wave representing a zone of transient combustion freely propagating in either the upstream or downstream direction within the porous medium [5].

Dixon et al. [6] studied the conversion of liquid heptane to syngas in a packed bed reactor containing alumina pellets. The heptane feed was vaporized with air. The experimental and numerical investigations focused on the effects of the equivalence ratio (φ) and the inlet velocity on the outlet composition. The equivalence ratio is defined as the ratio of the stoichiometric air flow rate and the actual air flow. With constant input velocity, the hydrogen production increased with an increase of equivalence ratio, and hydrogen conversion efficiency reached its maximum value when φ was approximately equal to 3.0. Tests at a constant equivalence ratio of 2.5 showed that the conversion efficiency increased with the inlet velocity, and at the highest velocity tested of 80 cm/s, the experimental values exceeded 80%. Similar trends were observed for carbon monoxide conversion and energy efficiencies, with maximum values that exceeded 90 and 80% respectively. Overall, the results indicated that favourable conditions for fuel reforming are with φ of 2.5–3.5, and showed that the inlet velocity has a significant effect on the performance. There was a substantial gain in efficiency with the increase in the inlet velocity, which was attributed to the increase in the temperature of the reactor.

The works of Pedersen-Mjaanes et al. [7] and Pastore and Mastorakos [8] on super-adiabatic combustion of liquids (methanol, octane and n-heptane, among others) in a two-layer porous burner with steady rich stabilized flames demonstrated the capacity to produce syngas rich in hydrogen. In particular, Pastore and Mastorakos [9] investigated the rich combustion of n-heptane, diesel oil, kerosene and rapeseed-oil methyl ester (RME) biodiesel, for the purpose of producing syngas for fuel cells applications, or for the enrichment of traditional combustion chambers. The rich flames were stabilized in a combustor of inert porous media with two-layers and were examined over a range of equivalence ratios and porous materials. The n-heptane was successfully reformed until a value of φ equal to 3.0, reaching a conversion efficiency (based on the lower heating value of H_2 and CO over the fuel input) up to 75% for a packed bed of alumina beads. Similarly, diesel, kerosene and biodiesel were reformed to syngas in a zirconia foam burner with conversion efficiency over 60%.

Others [1,10] reported research in non-catalytic filtrational combustion for the conversion to syngas of wet ethanol, jet-fuel (Jet-A) and butanol. The experimental and numerical results with wet ethanol (ethanol that has only been partially distilled and dehydrated) over a range of equivalence ratios, inlet velocities, and water fractions, indicated that wet ethanol can be effectively converted to syngas in a non-catalytic filtration reactor, thus negating the necessity of complete dehydration and distillation to dry ethanol, demonstrating that this fuel is a promising biological source for hydrogen. The results also showed that the conversion of ethanol to syngas by filtrational combustion is similar to the conversion of n-heptane and methane, in terms of the behaviour of the combustion as a function of the equivalence ratio and the inlet velocity. In the case of experimental research with Jet-A and butanol, the results showed that approximately 42% of the hydrogen of the Jet-A was converted to H_2 and that 56% of the carbon was converted to CO. The H_2 yield continued to increase with φ in the experiments with Jet-A, whereas with butanol the yields of H_2 and CO both reached a maximum within the operating range studied. The peak CO yield with butanol was 72% and for H_2 it was 43%. The main products were H_2 and CO, however, CH_4, C_2H_2 and C_2H_4 were also observed in considerable quantities for both fuels, especially in experiments with butanol at φ greater than 3.0.

Decalin is a two-fused ring cycloparaffin, which is found in liquid fuels (jet fuels, diesel). It is a model compound for bicyclic naphthenes found in jet fuels and coal-, oil-shale-, tar-sand derived fuels, and it is also a potential endothermic fuel for hypersonic flight [11]. The importance of decalin in this study lies in the fact that has structural proximity to the average chemical species that can be found in a heavy fuel oil [12] and because it has been found that in mixture (methylnaphthalene/decalin/cyclohexane/*n*-hexadecane) is a promising surrogate of this fuel in combustion process [13]. Moreover, the development of semi-detailed chemical kinetic reaction mechanisms, based on lumped reactions and species for simplified description of the formation of decomposition products, which includes both low- and high-temperature chemistry, allow to study the oxidation and pyrolysis of decalin on a wide range of conditions of pressure, equivalence ratio and temperatures [14].

The main objective of this work is to present a phenomenological model for rich combustion of heavy fuel oil No. 6 in a packed-bed reactor using decalin as a model compound, and to compare the results with some experimental values. We considered a simple kinetic global scheme for the partial oxidation reforming (POR), and perform a validation with experimental data of temperatures and concentrations of gaseous products for a reactor containing IPM. Equilibrium calculations were made using the lumped reaction mechanism developed for Dagaut et al. [14]. In the following, we first describe the experimental arrangement, then the mathematical model, and then some results and discussion.

Experimental equipment and procedure

Experiments were performed using heavy fuel oil No. 6 in a packed-bed reactor. Fig. 1 shows a diagram of the

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