



ELSEVIER

Available online at www.sciencedirect.com

ScienceDirect

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

Modeling hydrogen production in a catalytic-inert packed bed reactor by rich combustion of heavy fuel oil

J. Gómez ^a, J.P. Mmbaga ^c, R.E. Hayes ^{c,**}, M. Toledo ^{b,*}, F. Gracia ^a^a Department of Chemical Engineering and Biotechnology, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Beauchef 850, Santiago, Chile^b Department of Mechanical Engineering, Universidad Técnica Federico Santa María, Av. España 1680, Valparaíso, Chile^c Department of Chemical and Materials Engineering, University of Alberta, Edmonton, Alberta, Canada

ARTICLE INFO

Article history:

Received 15 September 2017

Received in revised form

8 December 2017

Accepted 9 December 2017

Available online xxx

Keywords:

Filtration combustion

Partial oxidation reforming

Catalytic cracking

Heterogeneous modeling

Decalin

Syngas

ABSTRACT

This work presents simulation results for the production of hydrogen by the rich combustion of heavy fuel oil in a dual zone packed bed reactor. The first zone provides catalytic-thermal cracking of the fuel and is followed by a second zone for partial oxidation reforming of the cracked products. The kinetic model for the heavy fuel oil reactions in the catalytic zone uses decalin as a model compound. The partial oxidation reforming zone uses model compounds for the product groups formed from decalin cracking, and uncracked decalin. The hybrid reactor model is compared to results from a model of an inert (non-catalytic) porous media reactor. The work considers equivalence ratios from 1 to 2, filtration velocities between 15.0 and 65.5 cm/s, heat loss from 10 to 108% and particle diameter between 3 and 7 mm, and evaluates their effect on conversion. The simulations with the hybrid reactor model, in slightly rich conditions (equivalence ratio = 1.3) and constant filtration velocity of 19.3 cm/s deliver maximum hydrogen production for an optimal length of the intermediate zone. Considering this optimization: the total energy conversion efficiencies improve with the increase of the equivalence ratio due to the presence of hydrocarbon species generated by the cracking process. It is observed that the hybrid reactor model makes a better use of vaporized fuel, compared to a model for an inert packed bed reactor, when the deposits of carbonaceous material in the latter exceed 7.4%.

© 2017 Hydrogen Energy Publications LLC. Published by Elsevier Ltd. All rights reserved.

Introduction

Hydrogen can be produced from many different sources by various methods. Some example technologies are: thermochemical splitting of water, catalytic steam reforming of

mixtures of bioglycerine and bioethanol, biomass fermentation, biophotolysis of water, low temperature catalytic gasification of fowl manure, electrochemical oxidation of urea and photocatalytic decomposition of H₂S [1]. In particular, hydrogen production from heavy hydrocarbons can be carried out by catalytic steam reforming, catalytic partial oxidation

* Corresponding author.

** Corresponding author.

E-mail addresses: bob.hayes@ualberta.ca (R.E. Hayes), mario.toledo@usm.cl (M. Toledo).<https://doi.org/10.1016/j.ijhydene.2017.12.056>

0360-3199/© 2017 Hydrogen Energy Publications LLC. Published by Elsevier Ltd. All rights reserved.

and autothermal reforming. At present, catalytic hydrocarbon reforming is the best-developed and most economical technique for hydrogen production [2]. It has also been possible to produce hydrogen through combustion in porous media using different configurations and fuels [3–9].

Porous combustion technology is a novel energy utilization process, environmentally benign, and efficient, located at the forefront of modern technological developments [10]. It corresponds to non-catalytic combustion with propagating wave-like high-temperature zones, which are established by heat recirculation within the porous bed (*filtration combustion*) and shows reaction fronts inside a porous matrix characterized by rapid exothermic reactions influenced by large interfacial heat transfer [11]. In particular, conversion to syngas has been successfully realized with liquid fuels by filtration reactors and other types of heat-recirculating reactors [8].

Recent studies of filtration combustion of liquid fuels to syngas have considered different kinetic approaches, with either overall or detailed mechanisms for specific model compounds. An experimental and numerical study of conversion of liquid heptane to syngas through non-catalytic combustion in a packed bed of alumina pellets used a mechanism of intermediate complexity for the computational results, composed of 107 species and 723 reactions to describe the high temperature oxidation and pyrolysis of *n*-heptane, iso-octane, and their mixtures [11,12]. The comparison of experimental and numerical results showed good agreement only for equivalence ratios less than 2.0, and between 2.0 and 3.0 numerical simulations gave significantly higher hydrocarbon than those measured in experiments. Another work on partial oxidation of diesel fuel in a porous reactor for the production of syngas used *n*-heptane as a diesel surrogate fuel. For these numerical investigations, the comprehensive mechanism of Curran et al. [13] was used in equilibrium and kinetic analyses. The results showed that the deviation between the measured and equilibrium concentrations were large for an excess air ratio lower than 0.45 due to the formation of CH₄, C₂H₂, soot, and other hydrocarbons, compared to the equilibrium H₂ and CO concentrations calculated using *n*-heptane surrogated fuel [14]. Recently, the work of Gómez et al. [15] on filtration combustion modeling of HFO to syngas production used the overall chemical kinetics model for partial oxidation of methane in inert porous media [16,17] and water gas shift reaction under non-catalytic conditions [18], combined with stoichiometric, chemical and physical properties for decalin as a model compound. Their numerical results showed a good agreement with experimental exhaust concentrations of H₂, and positive effects of the equivalence ratio (ϕ) and filtration velocity (v_{filt}) increase and heat losses reduction on the fuel conversion to H₂.

Decalin is widely used as a model compound for mixtures of commercial fuels such as diesel, jet fuel, and heavy fuel oil [19–22]. Decalin is a two-fused ring cycloparaffin and a model compound for bicyclic naphthenes found in jet fuels and coal-, oil-shale-, oil-sand derived fuels, and it is also a potential endothermic fuel for hypersonic flight [23]. Furthermore, it has structural proximity to the average chemical species that can be found in a typical heavy fuel oil [24]. Also, decalin is a possible compound representative of cyclo-alkanes present in diesel fuel [19]. It has been used in mixtures as a surrogate for

low-sulfur JP-8 in a study of autothermal reforming, with good correlation, in a three-component mixture of *n*-dodecane/decalin/toluene [20]. To emulate the fuel properties affecting the spray development and gas phase ignition of a conventional jet fuel, a mixture of *n*-dodecane/*iso*-cetane/decalin/toluene was used. The results showed good agreement for liquid density and volatility, important properties for spray predictions under engine conditions [21]. In regard to the combustion of HFO, it has been found that a mixture of composition methyl-naphthalene/decalin/cyclohexane/*n*-hexadecane is a promising surrogate of this fuel [22].

Concerning the production of synthesis gas from HFO using an inert porous medium reactor, practical experience indicates that a carbonaceous residue is formed in the packed bed, giving a lower efficiency [25]. An alternative to achieve a better fuel efficiency is to use a packed bed reactor of two zones in series, in which the first zone contains a packing of zeolite catalyst, performing a catalytic-thermal cracking of the premix rich air-fuel, which has previously been vaporized in an initial inert hot zone. The products from the cracking, along with excess fuel, can be processed in the second zone with an inert packed bed, where they are subjected to partial oxidation.

With regard to the catalytic cracking of HFO on zeolitic catalysts, Otterstedt et al. [26] studied the effect of added alumina to the matrices of cracking catalysts containing different types of zeolite Y on their cracking performance when processing a heavy vacuum gas oil feed (HVGO) and #6 Fuel Oil. The temperature of the reactor for fuel oil was 560 °C. They mentioned that #6 Fuel Oil was a considerably more difficult feed to crack, and concluded that for this feed, the alumina addition resulted in a higher conversion at the same catalyst to oil ratio, independent of the type of zeolite. This higher conversion was accompanied by a greater selectivity for coke and a lower selectivity for gasoline.

Since the results of modeling of filtration combustion of HFO using decalin as model compound were consistent with experiments [15], it is proposed to use decalin for modeling the catalytic cracking of the fuel. The study of Al-Sabawi and de Lasa [27] on the cracking of decalin on zeolites in industrial FCC conditions provides kinetic information that can be used to approximate the kinetic behavior of the reactive process in the first zone of the combined reactor. They found that decalin undergoes reactions such as ring opening, protolytic cracking, isomerization, hydrogen transfer and transalkylation. They proposed a heterogeneous kinetic model for decalin conversion that included thermal effects, adsorption and intrinsic catalytic reaction phenomena. It was determined that hydrogen transfer reactions were more pronounced and selectively favored against other reactions at lower reaction temperatures, while ring-opening and cracking reactions predominated at higher reaction temperatures.

This paper reports a modeling approach (named here as *Model C-I*) proposed for a catalytic-inert combined reactor used for the processing of #6 Fuel Oil in a packed-bed reactor using decalin as a model compound. Although this process has been proposed for the steam reforming of methane, it has not been discussed for the case of valorized liquid fuels. In the following, we first describe the mathematical model, and then some simulation results and discussion.

Download English Version:

<https://daneshyari.com/en/article/7707970>

Download Persian Version:

<https://daneshyari.com/article/7707970>

[Daneshyari.com](https://daneshyari.com)