

Recent advances in catalytic oxidation and reformation of jet fuels



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HIGHLIGHTS

- Review of catalytic conversion of JP-8 fuel over the last one decade is provided.
- Provided role of catalyst, support materials, and preparation methods on reforming.
- Sulfur tolerant catalysts and mechanisms of catalyst poisoning is poorly understood.
- Role of hydrocarbons present in jet fuels during fuel reforming remains a challenge.
- High fidelity numerical simulations limited to gas phase non-catalytic reforming.

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ABSTRACT

This paper provides a review of progress in catalytic conversion of JP-8 fuel and its surrogates made over the last decade. The effect of different types of catalyst and support materials, as well as different preparation methods, is discussed in detail. The derivation of kinetic models for computational studies is also examined. Particular attention is given to the development of sulfur tolerant catalysts and the mechanisms by which catalyst poisoning occurs, as this is an important obstacle to overcome for systems using sulfur-laden fuel. Suggestions for further research are offered.

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1. Introduction

Jet propellant-8 (JP-8) is a conventional petroleum-derived jet fuel used extensively as a logistic fuel by U.S. military. JP-8 contains a wide distribution of alkane, cycloalkane, and aromatic compounds, ranging from C_8 to C_{16} , as well as up to 3000 ppm by weight of sulfur [1]. Alternative jet fuels derived from methods such as Fischer–Tropsch synthesis and extraction from biomass have also been developed and shown to possess similar characteristics and performance as conventional JP-8 [2–8]. These alternative fuels tend to only contain paraffin species and negligible sulfur compounds. The complex nature of this JP-8, together with the fact that every batch has a different composition [1], makes it difficult to draw many meaningful conclusions from experimental work, and makes it almost impossible to develop a detailed kinetic model. As such, many researchers prefer to use surrogate fuels, which typically contain 1–3 different components (although more intricate ones can have more) that are representative of the fuel being studied. For JP-8, most surrogates contain a paraffin (typically dodecane), an aromatic (such as benzene, toluene, or xylene), and occasionally a cycloalkane, as these are the three primary classes of hydrocarbon found in the fuel [9].

The use of a catalyst during the conversion of liquid hydrocarbons offers several benefits. First, the primary function of a catalyst is to lower the activation energy needed to initiate combustion, thus allowing the reaction to ignite at a lower temperature, reducing the need for input power at startup. Stemming from this, catalytic reactions tend to proceed at lower temperatures than purely gas-phase reactions, which is favorable for portable power generation applications. Catalysts are also very active in determining the product selectivity of the reaction, so a system can be tailored to fit the individual needs of the user. To evaluate the effectiveness of a catalyst for JP-8 conversion, the effects of different types of hydrocarbons must be taken into consideration. To this end, extensive studies have been performed to examine the influence of different classes of hydrocarbons on catalytic performance and to optimize the reactor or operating conditions to meet the researchers' respective goals [10–16]. Small-scale catalytic systems utilizing logistic fuels can be used in a multitude of applications, including portable power generation [17,18] and fuel processing for fuel cells [19].

Several review papers exploring this topic have already been published [20–24]. These papers primarily concentrate on either a specific class of catalyst or a specific application. The current review provides a broader view of the topic, focusing on the characteristics of suitable catalysts, the development of kinetic models, and the investigation of sulfur-tolerant catalysts for use with JP-8 and its surrogates. Suggestions for further studies are also presented. There were some classical reviews [25,26] that offer board perspectives published in late 90s and early 2000s. The current review covers selected publication over the last decade. Most numerical simulation efforts deal with non-catalytic reforming and that also with gas phase only due to the complexity and extremely large number of reactions involved under reforming conditions as compared to combustion conditions. Numerical simulation of gas phase non-catalytic reforming is given by Kim and Dean [27]. This study used ANSYS Fluent v15 code wherein coupled CFD kinetics was used for the mixing region during autothermal reforming of diesel surrogate ($n\text{-}C_{12}H_{26}$) fuel with

limited number of chemical species included in the gas phase mechanism assuming complete fuel evaporation. Catalytic reactions are often modeled as lumped reactions. However, there are no real validated papers that deal with simulation of both homogeneous and heterogeneous catalytic reforming.

2. Catalysts

2.1. Catalyst materials

2.1.1. Supported metals

The most common type of catalyst for oxidation or reformation of jet fuels and other liquid hydrocarbons is a supported metal, in which a support (either inert or catalytic) is coated with an active metal species. Depositing the metal particles on the support allows for greater particle dispersion and thus higher catalytic activity. Different metals have different catalytic properties. Santos et al. [28] compared the activity of Pt, Pd, Ir, Rh, and Au catalysts supported on TiO_2 for toluene oxidation. They reported the following trend in activity: $Pt > Pd \gg Rh \cong Ir \gg Au$. This was explained in terms of the oxidation method of toluene on noble metals—each metal has a dissociative chemisorption energy for O_2 . At a given temperature the specific activities of each metal as a function of oxygen chemisorption energy form a volcano plot; metals with very low or very high chemisorption energies have low activities due to lowered capability for adsorption/desorption from the catalyst surface, and metals with a median value have high activities due to a functional balance of adsorption/desorption. The volcano plot for toluene and ethanol from this study is presented in Fig. 1. Pt and Rh catalysts were also compared in terms of activity for CPOX of decane to form H_2 and olefins in an earlier study [29]. For this application, Rh had significantly higher H_2 and olefin production; Pt produced hardly any H_2 . Kim [30] studied Cu, Fe, Mn, V, Mo, Co, Ni, and Zn catalysts supported on $\gamma\text{-}Al_2O_3$ for the oxidation

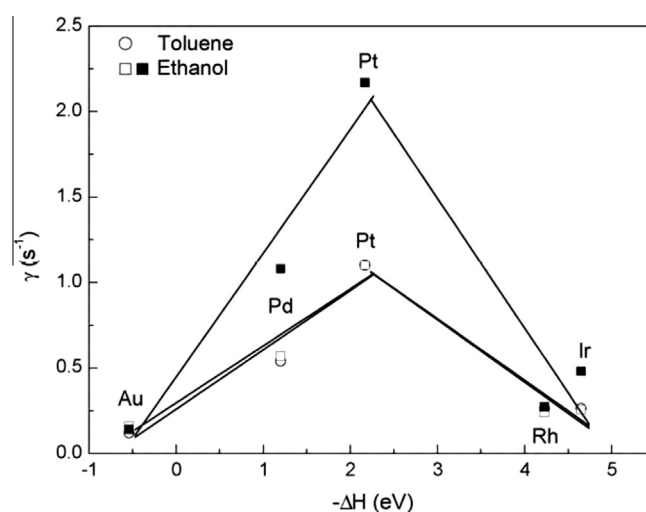


Fig. 1. Volcano-type plot indicating the specific activity (γ) at 285 °C in VOC oxidation as a function of oxygen dissociative chemisorption energies ($-\Delta H$) on metals. The filled symbols represent the catalysts prepared by incipient wetness impregnation, while the empty symbols represent the catalysts prepared by liquid phase reduction deposition [20].

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