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The impact of fuel evaporation on the gas-phase kinetics in the mixing region of a diesel autothermal reformer

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ABSTRACT

Autothermal reforming is a promising technology to produce syngas from diesel fuel. However, the mixing of liquid diesel fuel with high temperature streams of steam and oxygen presents a challenge: how to avoid formation of ethylene, a likely deposit precursor, in the region upstream of the catalyst bed. This work describes a coupled CFD-kinetics study in the mixing region of a diesel autothermal reformer that considers: (1) an atomizer model to explicitly account for fuel evaporation, (2) *n*-dodecane as a surrogate diesel fuel, (3) oxygen as the oxidant instead of air. The predictions indicate unacceptable levels of ethylene (>0.1 mol%) will be present at the mixer exit if the mixer gas temperature is greater than ~350 °C. This temperature is likely to be too low for proper catalyst performance. Thus this analysis suggests that either improved mixer designs or a different choice of catalyst might be required to achieve suitable diesel autothermal reforming performance.

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Introduction

Diesel reforming technology has been proposed as a hydrogen production method for portable fuel cell applications due to the high energy density of diesel fuel. Autothermal reforming is considered to be the most appropriate method to reform liquid fuels, since it shows high conversion of heavier hydrocarbons and aromatic components in fuels [1,2] and also high reforming efficiency without an external heat supply [1–3]. Since autothermal reforming uses O₂ as one of reforming agents, there is the potential of unwanted gas-phase reactions in the mixing region prior to a reforming catalyst [4]. C₂H₄ is one of side products from such gas-phase

reactions, which is known to be a serious deposit precursor [5,6]. Therefore, one major issue in developing high-performance reformers for liquid fuels is to avoid substantial gas-phase reaction that could lead to significant C₂H₄ production during mixture preparation. The mixer design is complicated by the conflicting requirements of minimizing the time to suppress undesirable gas-phase reactions while allowing sufficient time for the reactants to be completely mixed so that there are uniform concentration and temperature profiles at the entrance plane of the catalyst. In addition to this uniformity of profiles, the temperature must be sufficiently high to allow the catalytic reactions to proceed. Thus the overall mixer design will depend upon the minimum operating temperature of the catalyst.

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In a previous work, a coupled CFD-kinetics analysis was performed to investigate the gas-phase reactions in the mixing region of a diesel reformer, using $n\text{-C}_7\text{H}_{16}$ as a surrogate fuel [7]. That work demonstrated the counter-intuitive result that mixing the reactants at relatively high temperatures ($\sim 550^\circ\text{C}$) decreased the rate of production of C_2H_4 . This was due to the unusual (but well-characterized) negative temperature coefficient (NTC) behavior during alkane oxidation; the oxidation rate decreases as the temperature increases above $\sim 450^\circ\text{C}$ due to shifting equilibria in the system. However, that work assumed that the fuel was pre-vaporized. As a result, the effective residence time for fuel vapor was increased, and the decrease in temperature that would accompany fuel evaporation was not accounted for. Another constraint in that analysis was the use of $n\text{-C}_7\text{H}_{16}$ as a surrogate fuel, due to the limitation in the number of chemical species that could be included in the chemical mechanism in the CFD analysis using the ANSYS Fluent v13 software package available at that time. Thus subtleties in the kinetics that might be present with a larger alkane were not considered.

The present work extends the previous coupled CFD-kinetics analysis in the mixing region of diesel autothermal reforming system in two ways: (1) the fuel evaporation process is accounted by employing an atomizer model. A twin-fluid nozzle is chosen for this work, since it was used in previous successful demonstrations [2,8]. (2) A more complex diesel surrogate, $n\text{-C}_{12}\text{H}_{26}$, can be used since a newer version of ANSYS Fluent (v15) removed the limitation in the number of chemical species that can be included in the mechanism. The use of this alkane surrogate can be justified since the aromatics present in diesel fuel generally have lower gas-phase reactivity under the conditions encountered in the mixing region. The composition of reforming agents is also changed. In general, air is used as O_2 source, but this work assumes that an aqueous hydrogen peroxide solution is source of both O_2 and H_2O . Such a source might be for applications where air is not available. The hydrogen peroxide is considered to be completely converted to H_2O and O_2 before entering the mixing region. Therefore, the only difference from the conventional autothermal reforming is the absence of N_2 . It should be mentioned that the time required for C_2H_4 to reach 0.1 mol% with $n\text{-C}_{12}\text{H}_{26}$ is significantly less in the NTC region without N_2 dilution, as shown in Fig. 1. Thus the no N_2 dilution case makes it more difficult to avoid C_2H_4 formation within the mixing region. The detailed discussion on the use of this unusual reforming agent is beyond the scope of this work.

The results show that explicitly accounting for fuel evaporation with a more complex surrogate, $n\text{-C}_{12}\text{H}_{26}$, significantly changes the model predictions with the result that C_2H_4 formation is more likely. This increase is the result of two effects: (1) The fuel vapor initially passes through the high-reactivity (low temperature) region for a sufficient time to generate some C_2H_4 via the oxidation pathway. (2) As the vapor then passes into the higher temperature regions within the mixer, the high temperature pyrolytic pathway becomes important as a source of C_2H_4 . As a result, the reactant mixing at relatively high temperature ($\sim 550^\circ\text{C}$) would be not advantageous, unlike the conclusions of the previous investigation [7]. Another reason that this work predicts different results from the previous work is the use of $n\text{-C}_{12}\text{H}_{26}$ as a surrogate fuel,

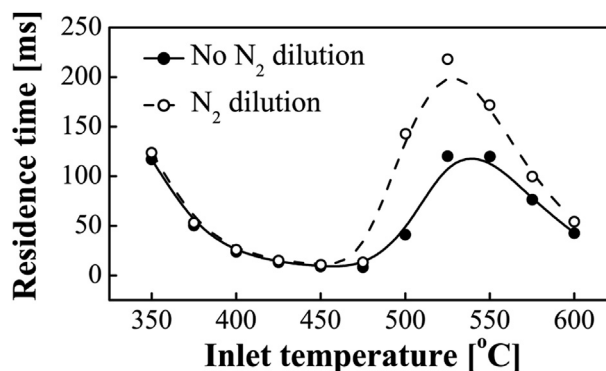


Fig. 1 – Comparison of adiabatic plug-flow predictions on the residence time required for C_2H_4 to reach 0.1 mol%, with and without N_2 dilution. The reaction mechanism of $n\text{-C}_{12}\text{H}_{26}$ is from the reference [9]. The lines are added to guide the eye.

which shows much less NTC behavior than $n\text{-C}_7\text{H}_{16}$ with respect to C_2H_4 production. Therefore, significant C_2H_4 generation is unavoidable with the current mixer design unless the temperature in the mixing region is maintained less than 350°C .

Model description

Geometric description

A simple design of the reactant mixer upstream of a reforming catalyst for 1kW_e -class diesel reformer has been suggested for this study (Fig. 2). The conceptual design and the dimensions of the reactor is based on previous work [2]. This design has been proven to be reliable for long-term operation since it was operated continuously for 250 h in the previous work. A liquid surrogate fuel, $n\text{-C}_{12}\text{H}_{26}$, and a gaseous mixture of H_2O and O_2 are supplied to the reactor. A twin-fluid nozzle (SU1A, Spraying Systems Co.) is used for fuel injection and atomization, since this nozzle was used in previous successful demonstrations [2,8]. It is mounted at one end of the reactor. The liquid fuel and a portion of the gaseous mixture is supplied to the nozzle and the remaining portion of the gaseous mixture is supplied downstream. In the original design, this secondary stream was supplied through a single pipe, but it has been modified to be supplied through the finely perforated sidewall

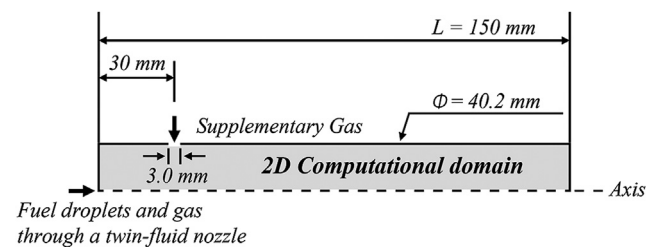


Fig. 2 – 2D-computational domain of the mixing region of 1kW_e -class diesel reformer.

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