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A PFA method for the reduction of Iso-octane

Naman Sharma
Department of Mechanical Engineering, Colorado State University, USA
Email: nmnsharma27@gmail.com

Abstract---- The depleting fossil fuel is raising concern for the coming future. To overcome this concern more research is being directed towards sustainability. One such area is Biodiesel, which can be sustained for the upcoming future. However, there are problems associated with Biodiesels such as its poor cold flow property and poor oxidative stability. Also, combustion of biodiesel is of paramount importance. Nowadays blends like B20 which is 20% biodiesel and 80 % diesel are used directly in an engine with little modifications. Study of reduced Iso-octane mechanism is the focus of this study. This paper takes isooctane as a surrogate to biodiesel for ignition delay study and early CO2 formation.

Keywords—-Biodiesel, Isooctane, Cold flow properties.

1. INTRODUCTION

The rapid decline in oil reserves and daily increase in dependency on fossil fuels has forced us to look for alternative energy sources. One of many such sources is the use of Biodiesel. Biodiesel is emerging as one of the most prominent fuels in the near future. Biodiesel is obtained from lipid materials such as vegetable oils and animal fats. It is defined as the fatty acid alkyl esters of edible oils, non-edible oils, animal fats or waste oils. The main process for producing biodiesel is the transesterification reaction, which consists of an alcoholysis of tri- glycerides to obtain methyl esters and glycerol as a by-product. The composition largely influences the critical parameters of the biodiesel. It is renewable, biodegradable and nontoxic, has low emission profiles and so is environmentally advantageous [1]. Biodiesel possesses inherent lubricity property and a relatively high flash point and reduces most of the exhaust emissions in comparison to petrodiesel. Therefore it is a technically competitive and environmentally friendly alternative to conventional fossil-derived diesel fuel for use in compression-ignition engines [2].

There are two major problems related to using of biodiesel as fuel these are its oxidation stability and cold flow performance.

1. Biodiesel consists of long chain fatty acid esters which may contain more or less unsaturated fatty acids which are prone to oxidation.

Biodiesel stability includes oxidation stability, storage stability and thermal stability accelerated by exposure to air during storage. Oxidation instability can lead to the formation of oxidation products like aldehydes, alcohols, shorter chain carboxylic acids, insoluble, gum and sediment in the biodiesel.

Thermal instability is concerned with the increased rate of oxidation at a higher temperature, which in turn, increases the weight of oil and fat due to the formation of insoluble saturated fatty acids.

Storage stability is the ability of liquid fuel to resist change in its physical and chemical characteristics brought about by its interaction with its environment and may be affected by interaction with contaminants, light, factors causing sediment formation, changes in color and other changes that reduce the clarity of the fuel. These fuel instabilities result in the formation of undesirable substances in biodiesel and its blends beyond acceptable quantities as per required specifications and when such fuel is used in the engine, it impairs the engine performance due to fuel filter plugging, injector fouling, deposit formation in engine combustion chamber and various components of the fuel system. Settling solid residues were found to clog fuel filters in vehicles. Therefore it is generally suggested that Biodiesel, not more than

2. Another problem is when biodiesel is left unattended (overnight) in a cold temperature it results in the formation of crystals or solid wax in the fuel. This results in plugging of filters in the engines. The temperature at which fuel filter plugging occurs varies from fuel to fuel depending on the composition of the fuel. However, this temperature is higher for biodiesel than petroleum diesel, for example, palm oil biodiesel will start to crystallize at about 16°C and will form a gel at about 12°C. this makes biodiesel not favorable in cold weather. In cold climate, it will be difficult to operate the vehicle because fuel will lose its flowability and there will be fuel starvation in the engine. The cold flow properties of biodiesel dictate that the length of the hydrocarbon chains and the presence of unsaturated structures significantly affect the low-temperature properties of biodiesel.

The present work focuses on the study of reduction of Iso-octane mechanism. Iso-octane shows the same Biodiesel characteristic at low temperature. Even LLNL has used same Iso-octane mechanism with other mechanisms to develop Biodiesel surrogate. [10]

[3] have used second generation biodiesel with diesel blends to study the combustion and emission characteristics. The result that came out shows

decreases in ignition delay with an increase in Blend ratio. The best result was given by IV_B20 blending fuel.

However, When [4] uses alcohol (ethanol or butanol) blends with biodiesel there was an increase in ignition delay timings.

[5] have similarly used ethanol blend with biodiesel and there was an increase in ignition delay as seen by the previous researcher.

[6] used Biodiesel blend with petro blends and there was no such significant change in ignition delay.

2. NUMERICAL METHODS

2.1 CHEMKINTM

CHEMKINTM is a software tool that helps in understanding the kinetics of fuels during combustion processes. CHEMKINTM has the ability to solve thousand of reactions and can help us to give a good idea of what is going around in the process. For this study, CHEMKINTM II software is used to study ignition profile, CO2 formation in NTC regime and flame measurements.

2.2 Iso-octane mechanism

Iso-octane version2 developed by Lawrence Livermore National Laboratory is the mechanism of my study. IC8H18 is being used because it shows the same unique property as of biodiesel at low temperatures, which is the production of early CO2 [10].

2.3 Reduction mechanism for Iso-octane

It has been reviewed that Iso-octane mechanism has got 857 species and 3606 reactions [7]. It is very unlikely to study those many reactions. The skeletal reduction is typically the first step of mechanism reduction, where species and reactions are removed over the range of conditions of interest (e.g. pressure, temperature, and equivalence ratio) from the detailed mechanism.

The DRG method has recently been shown to be particularly applicable to efficiently and reliably reduce large reaction mechanisms. In DRG, the coupling of species is mapped on a directed graph, which is then analyzed to find unimportant species for removal. Recently, further development of this method has branched into two directions: (a) DRG-aided sensitivity analysis (DRGASA), which performs sensitivity analysis on species not removed by DRG to further reduce the mechanism, and (b) DRG with error propagation (DRGEP), which considers the propagation of species coupling down reaction pathways. (c) A combination of both approach DRGASA and DRGEP has been used by [8]. It is illustrated that this combined approach overcomes the weaknesses of the two individual methods.

[9] DRG method-In this method interaction coefficient found out using a formula and is compared with a threshold value (given initial value) If the reaction coefficient is less than the threshold value then the relationship is considered negligible. However, the major drawback of this method is that only first generation is considered.

DRGEP method improves over DRG method considers second generation and much more. It first finds reaction flux for production and consumption. The interaction coefficient formula can be used when a third reactant species is introduced. For comparison, one threshold value is selected for comparison.

PFA is the advancement of the above method. While transforming from one species to another following an intermediate species. It also accounts for how much species is actually converted. PFA is very good method than DRG and DRGEP because it calculates Reaction path flux more accurately. [11]

For this study, Iso-octane mechanism was used for reduction of 857 species and 3606 reactions into 154 species for phi=1, 136 for phi=0.5 and 153 species for phi=2. The pressure values for reduction were (1,5,10 atm) and temperature values were (600,700,800 K). Since no flame study was done, the senkin data was taken instead of PSR data.

3. RESULTS AND DISCUSSIONS

Ignition and mole fraction of CO2 data before and after reduction

The reduced mechanism was run in CHEMKINTM II to get ignition data and mole fraction of CO2. This data is then compared with a detailed mechanism to check the authenticity of reduction. Fig. 1,2,3,4 shows clearly that the reduction was a success without much deviation in the ignition as well as CO2 data.

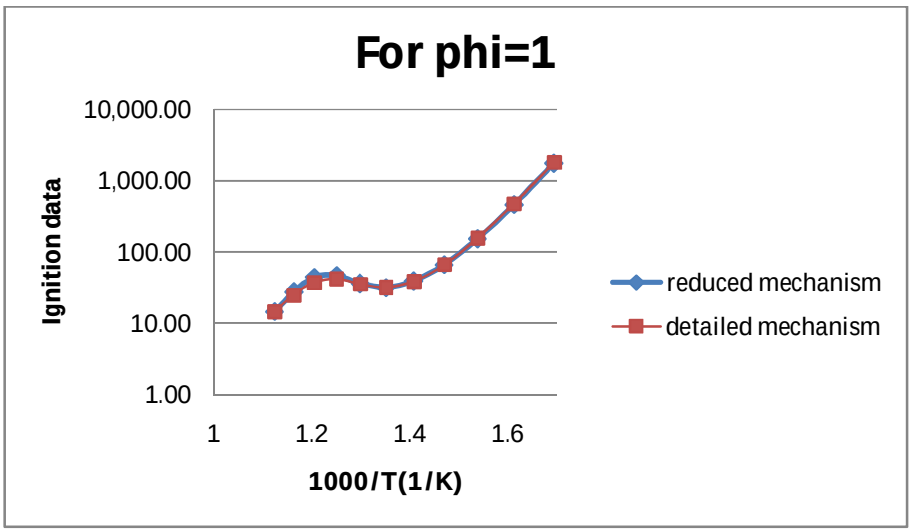

Fig. 1. Ignition data with NTC region for phi=1

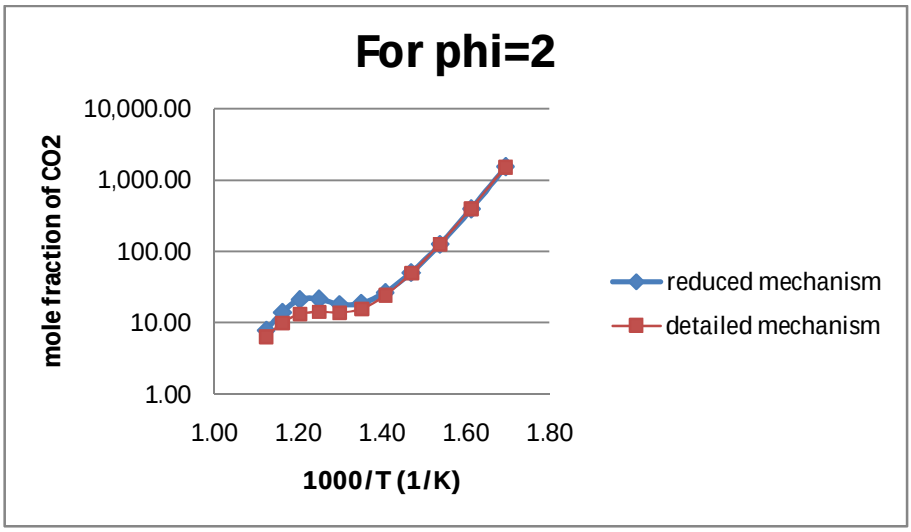

Fig. 2. Ignition data with NTC region for phi=2

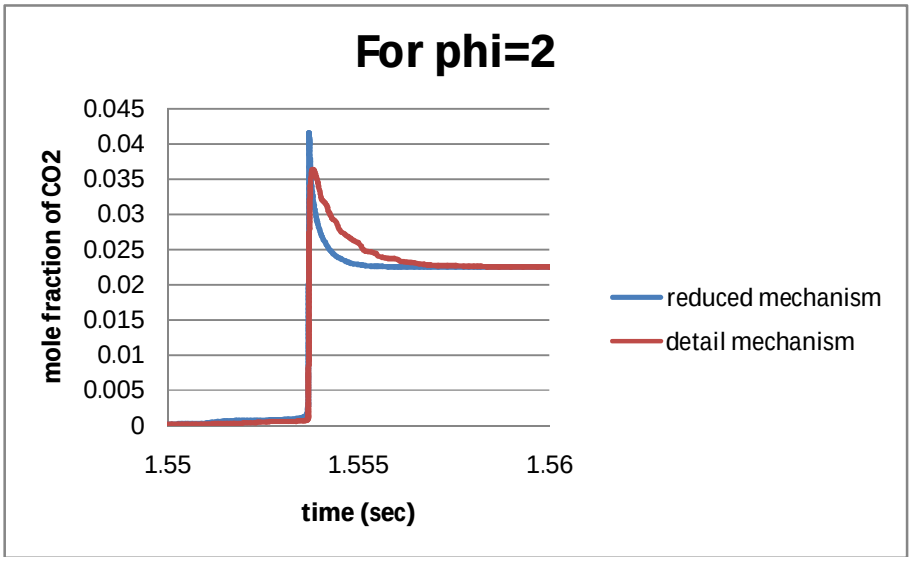

Fig. 3. Mole fraction of CO_2 for phi=2

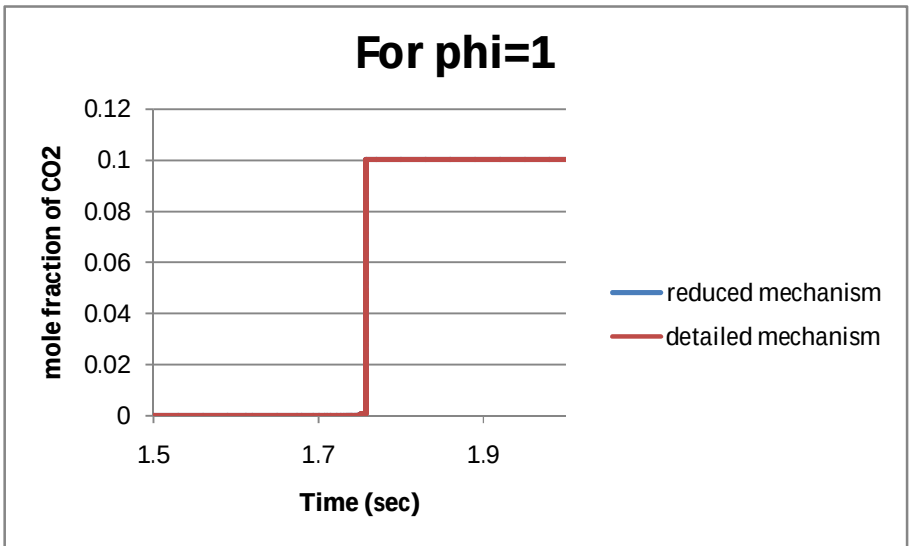

Fig. 4. Mole fraction of CO_2 for phi=1

4. Conclusion

The result of this study looks promising without much deviation in both the ignition and CO2 profiles. This shows the PFA method developed by Dr. Ju at Princeton University is promising. However, this software has one limitation. Unlike other softwares, this software does not run without transport data. Since the mechanism is chosen previously for study does not come with transport data. For that reason, the mechanism was changed to Iso-octane instead of Biodiesel surrogate. Also, this data should be complete for all species for a successful run.

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