ABSTRACT

Practical fuels are complex mixtures of hydrocarbons. In order to investigate the combustion of these fuels, it is necessary to propose and validate kinetic reaction mechanisms in simple and well-defined laboratory conditions for the combustion of selected simple hydrocarbons representing the major components of practical fuels. A practical fuel will then be represented in the model by a simple mixture of hydrocarbons called the reference fuel or model-fuel. In the present research project, investigations on the reaction kinetics of iso-octane have been done.

The critical problems of engines are the control of ignition timing and reducing the formation of pollutants. In order to investigate and solve these problems the kinetic reaction mechanism must predict, first, the ignition times of the fuels and the formation of precursors to emission. Iso-octane is selected as reference fuel since it can be used successfully for the investigation of the main properties during gasoline combustion.

Because of the exponential increase in the number of automobiles and the other propelling devices, the pollution of atmospheric air is of great concern. Hence in this study, importance is also given to the identification of reaction pathways of the heavy hydrocarbon fuels which are responsible for the production of harmful emissions.
Iso-octane (2,2,4 trimethylpentane), a primary reference fuel for octane rating in spark ignition engines, has drawn considerable interest as a model hydrocarbon fuel for branched alkane components found in gasoline. Due to its relevance to practical liquid fuels, iso-octane has been the subject of many experimental and kinetic modeling studies. Experimental investigations of iso-octane oxidation and ignition have been carried out in shock tubes, rapid compression machine, jet strived reactors and flow reactors. Kinetic modeling is extremely useful, as actual experiments of this kind are difficult and very expensive.

The goal of the present study is to establish the understanding of premixed combustion systems and to determine the relationship between auto ignition delay time, soot formation and emissions at various temperatures, pressures, and equivalence ratios using kinetic modeling.

In the construction of a chemical kinetic model, a number of assumptions have to be made. In fact the assumptions are made with the conditions simulated corresponding to those available in the experimental side. The complete reaction mechanism (994 reactions and 201 species) which involve in the combustion of iso-octane is proposed and validated with LLNL detailed mechanism. Initially 3606 elementary reactions and 857 species were chosen and through a sensitivity analysis the simplified mechanism is arrived.
Cantera, an object oriented software for reacting flows is used in the present investigations.

Reaction models were used for predicting the concentrations, pressure and temperature profiles. Ignition delay times were computed using the OH criterion and from temperature and pressure profiles. All these results were within 10% agreement with experimental values. Over the range of initial conditions of these studies, the proposed reaction model predicts ignition delay which agrees well with the present results and other similar published data.

The kinetic model was subjected to a detailed sensitivity analysis from which the relative contribution of each reaction and the significant reactions are identified. It is observed that the unimolecular decomposition of the fuel is the most significant reaction in all the reactions. Also, in lean mixtures, H and CH₃ are the abstracting species. At stoichiometric conditions the species H, OH and CH₃ are significant.

The kinetic profiles of this fuel indicates that the concentration of intermediate species grow at faster rate for lean mixtures as a consequence of which the ignition delay is shortened. On account of the higher levels of OH, its reaction with other species are predominant whereas in rich conditions the emphasis shifts to H and CH₃. Ignition delay times are computed at varying equivalence ratios. The initial conditions are similar to the SI engine conditions and shock tube conditions.
In addition to establishing a compact reaction mechanism for the fuel iso-octane, the relative significance of each elementary reaction, the conditions for emission of CO and soot beyond permissible levels have also been determined. The mandatory permissible level of CO for automobile emission being 3% by volume, the rich limits of stoichiometry (Φ=2.0) for this is determined from the graph as less than 1% by volume.

Even though the experimental measurements of soot is very difficult, the theory of growth of soot formation kinetics have been explained and profiles of the species which act as precursors to soot like CH, C_2H, C_2H_2, C_3H_3, C_3H_4, C_3H_6 and C_4H_6 have been determined from the validated mathematical model.