A simplified chemical kinetic mechanism has been developed to simulate iso-octane combustion over a wide range of temperature, pressure and equivalence ratio conditions. This mechanism is based on the LLNL (Lawrence Livermore National Laboratory) detailed mechanism of iso-octane combustion. The overall reactivity of iso-octane results obtained is found to be agreeable with previous studies. In addition, an experimentally quantified intermediate species profile in shock tube studies is well reproduced by the model, indicating that the chemical pathways leading to their formation are well explored.

The proposed plausible chemical kinetic model for the combustion of iso-octane mechanism consists of 994 elementary reactions with 201 species. This reaction mechanism has been validated with LLNL detailed mechanism and those available in literature. This model was also found to yield ignition delay values for these fuels that are close to the measured ones for the specified range of temperatures, pressures, equivalence ratios and diluents.

For all the cases of iso-octane combustion, increase in the initial pressure and temperature cause a reduction in the ignition delay time. When equivalence ratios were reduced the induction periods also get reduced.
Probable thermal and kinetic explanations are offered for the variations in ignition delay times for varying diluent concentrations, stoichiometry, pressures and temperatures.

The reaction models were used for predicting the concentration of the species pressure and temperature profiles during the reaction time. Ignition delay times were computed using the OH criterion and from temperature and pressure profiles. All these results were within 10% agreement with the experimental observations of other researchers also. Over the range of initial conditions of these studies, the proposed reaction model predict ignition delay which agree 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 CH$_3$ are seen as the abstracting species. At stoichiometric conditions the species H, OH and CH$_3$ are significant.

The kinetic profiles of C$_8$H$_{18}$ combustion 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 higher levels of OH, its reaction with other species are predominant whereas in rich conditions the emphasis shifts to H and CH$_3$. Ignition delay times are
computed at varying equivalence ratios. The initial conditions are nearly equal to the SI engine conditions and shock tube conditions.

Investigations were carried out to predict the emissions like CO, CO$_2$ and CH in iso-octane at varying equivalence ratios from 0.5 to 2.0 and N$_2$ dilutions from 79% to 90% corresponding to conditions considered in shock tube and IC engine conditions. The influence of diluent gases on ignition times should be considered when designing shock tube experiments, comparing shock tube results to kinetic measurements made in other reactors, and with experiments and simulations.

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 been determined. The mandatory permissible level of CO for automobile emission being 3% by volume, the rich limits of stoichiometry ($\Phi=2.0$) 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$_2$H, C$_2$H$_2$, C$_3$H$_5$, C$_3$H$_4$, C$_3$H$_6$ and C$_4$H$_6$ have been determined from the validated mathematical model.
The proposed reaction mechanism is an accurate description of the major chain branching reaction paths and those kinetic processes which compete with the chain branching paths. In the present mechanism, the production and decomposition reactions of ketohydroperoxide molecules were found to provide the important low temperature chain branching, and the hydroperoxyalkyl decomposition reactions provide the major competition.

The model and the accompanying sensitivity analysis have shown the reaction pathways which are particularly important in each regime of pressure, temperature and equivalence ratio. Sensitivity analysis exhibits the importance of HO$_2$ creation and removal for predicting ignition times.

Comparison of measurements made for mixtures containing nitrogen as the diluent gas allow for an assessment of the influence of diluent gas on ignition time. The higher heat capacity of nitrogen results in measured ignition times that are longer, for most of the conditions studied, than those measured for other mixtures. Simulations performed using the other mechanisms predict that ignition times are in good agreement with the measurements on iso-octane shock tube ignition.
The mathematical model proposed can be reasonably used by practicing engineers and scientists for predicting desired values of temperature, pressure, ignition delay times and concentration profiles at any other initial conditions in the range of conditions viz. Temperature: 600 to 1200K, Pressure:10 to 40atm, \( \Phi \): 0.5 to 2.0, Diluent: 79\% to 95\%.

The difference between LLNL results and present results is due to the kinetic data used in the Cantera Software. The rate constant values are not taken from literature.