21st Australasian Fluid Mechanics Conference
Adelaide, Australia
10-13 December 2018

Numerical Investigation of Autoignition of Singlecomponent and Multicomponent surrogate of Diesel fuel

Anirudh Singh[1] and Amit Pal[1]

[1]Department of Mechanical Engineering
Delhi Technological University, Delhi 42, India

Abstract

This paper deals with designing of a three-dimensional computational model of an ignition quality tester and incorporating physical properties of surrogate fuel such as density, enthalpy, boiling point as a function of temperature in CONVERGE CFD to accurately and efficiently reproduce the ignition behaviour of single and multi-component surrogate of diesel fuel under different temperatures. N-Heptane is a most common diesel fuel surrogates and is also used for validating ignition quality tester. The pressure inside the chamber was fixed at 2.1MPa and the simulations were carried out at a chamber temperature of 770K, 800K, 830K and 860K. The collision, coalescence and evaporation of the fuel droplets was modelled using Patterson and Reitz-Helmholtz Rayleigh-Taylor (KH-RT) model. Skeletal chemical mechanism consisting of total 42 species and 168 reactions was used for combustion modelling of n-heptane and a reduced chemical mechanism consisting of 163 species and 887 reactions was used for determining the ignition delay for the multicomponent surrogate (n-dodecane/m-xylene) of diesel fuel to reduce the computational load. The various spray parameters like Sauter mean diameter, spray tip penetration length and vapor penetration were studied in all cases. The results show that the total ignition delay increases with the decrease in the chamber temperature. Also, it was observed that the chamber temperature has more effect on spray tip penetration over vapor penetration.

Introduction

Ignition quality of the diesel-type fuels is defined by its cetane number which can be determined either by engine-based cetane number testing methods or by non-engine-based ignitability testing methods. While the reliable measurements of these biogenic fuels have not been possible by the engine-based test methods [4], non-engine test methods like Ignition quality tester proves to be very accurate in determining the ignition quality of diesel and alternative diesel fuels with high repeatability and reproducibility.

Ignition quality tester is a bench-scale in which combustion of fuel takes place in a defined volume (0.21L) and contains a spray injection system designed for direct measurement of liquid fuel ignition delay. Ignition quality tester determines the ignition delay by measuring the time interval between the SOI (start of injection) and SOC (start of combustion) and for the measured ignition delay time, DCN (derived cetane number) is estimated using a standard correlation determined according to ASTM D6890-10a.

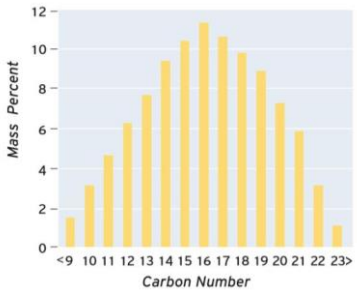

Figure 1. Carbon Number Distribution of 2-D Diesel Fuel

Diesel fuel composition

Diesel is a mixture of thousands of hydrocarbons mostly with carbon number between 10 and 22. The carbon number distribution for No. 2-D diesel fuel can be seen in Fig. 1. Most of these compounds are members of paraffin, naphthenic, or aromatic class of hydrocarbon with different chemical and physical properties [3] and thus development of chemical kinetic model for diesel is a difficult task due to its complex composition. To solve this problem, surrogate fuel with similar physical and combustion properties are develop which are used to simulate combustion and spray process of these complex fuels and hence reduce the computational time drastically.

Many researchers have tried to study the behaviour of n-heptane, n-decane, n-tetradecane and n-hexadecane under various pressure and temperature conditions as a possible surrogate for diesel fuel [7,8]. N-Heptane is most common diesel fuel surrogates and is also used for validating IQT (ignition quality tester). Numerous reduced chemical mechanisms are available in the literatures that have been validated experimentally in the shock tube experiments. Very less information is available on the how these surrogates behave under various temperature and pressure conditions.

This paper deals with a temperature sweep test conducted computationally on n-heptane and a multicomponent surrogate with a composition of 77% of n-dodecane and 23% m-xylene by volume to determine their behaviour under different temperature at a constant chamber pressure of 2.1MPa.

Methodology

A 3D model of high pressure and high temperature finite volume chamber was created in CONVERGE which can be seen in fig. 2. The pressure inside the chamber was fixed at 2.1MPa and the simulations were carried out at a chamber temperature of 770K, 800K, 830K and 860K. Thus, in total 4 simulations were carried on n-heptane and similarly another 4 simulations were carried for multicomponent fuel surrogate at an injection pressure of 20MPa and injection pulse width of 1.44ms.

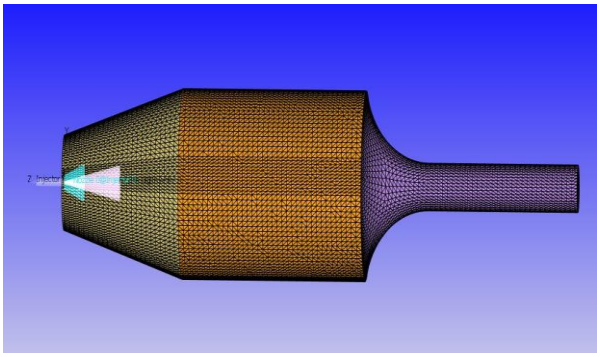

Figure 2. 3D model of ignition quality tester. Here the surface triangles should not be confused with the computational mesh.

Mesh Parameters

A three-dimensional computational model of ignition quality tester was developed on CONVERGE CFD to accurately and efficiently reproduce the ignition behaviour of single component surrogate of diesel fuel. CONVERGE uses cutcell cartesian method for mesh generation. The mesh generation process in CONVERGE is completely automatic and requires negligible human intervention for defining some basic mesh parameters like base mesh size, maximum embedding level etc.

All the simulations were carried with a base grid size of 4mm in all three directions and an adaptive mesh refinement of Level-2 based on velocity and temperature changes inside the combustion domain was employed. Adaptive mesh refinement is a very convenient technique to controls the number of elements and to provide refinement in selective areas where physical properties changes at a very fast rate. Along with the adaptive mesh refinement, a fixed embedding at a scale of 2 was also employed at the nozzle exit to resolve complex flow behaviour of spray in that region. The fixed embedding near the injector nozzle exit can be seen in the fig. 3.

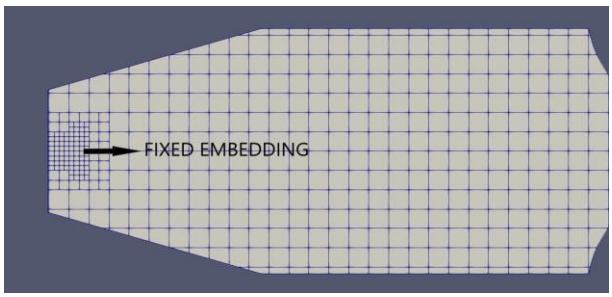

Figure 3. Fixed embedding near the injector nozzle exit

Spray Modeling and Chemical Kinetics

For liquid sprays, CONVERGE uses the Lagrangian solver to model discrete parcels and the Eulerian solver to model the continuous fluid domain. The fuel is introduced into the domain from the injector in form of parcels, that is a collection of drops. Each parcel represents a group of identical drops with same radius, velocity, temperature, etc. solves for radius, velocity, etc. The software uses sub-grid models for the spray processes that occur on length scales that are too small to be resolved to solve for radius, velocity, etc. on a per-parcel basis rather than a per-drop basis.

The effects of turbulence due to fuel spray in the constant volume chamber of the ignition quality tester is moderate compared to those in reciprocating engine so its effect was accounted using a K-epsilon turbulence model. Physical properties of the surrogates such as density, enthalpy, boiling point as a function of temperature were incorporated to mimic the droplet collision, coalescence and evaporation of the fuel droplets using Patterson and Reitz-Helmholtz Rayleigh-Taylor (KH-RT) model which represent the spray breakup process more accurately at higher pressure [6].

The drag on the fuel droplets was accounted by dynamic drag model [5]. The droplet collision and coalescence phenomenon play a vital role in obtaining accurate results in case of dense sprays. The spray and vapor penetration length were defined as distance from the nozzle tip to axial location of 95% and 1% of fuel mass fraction respectively.

The overall ignition delay of single component (n-heptane) surrogate in IQT is dominated by chemical kinetics over the spray physics and thus reduced/skeletal chemical mechanism consisting of total 42 species and 168 reactions were used for n-heptane and similarly another reduced chemical mechanism consisting of 163 species and 887 reactions was used for determining the ignition delay for the multicomponent surrogate of diesel fuel to reduce the computational time[2]. The injector modelled for the simulations is a saturation type fuel injector [1] and the variation of rate shape with the time(s) can be seen in fig. 4.

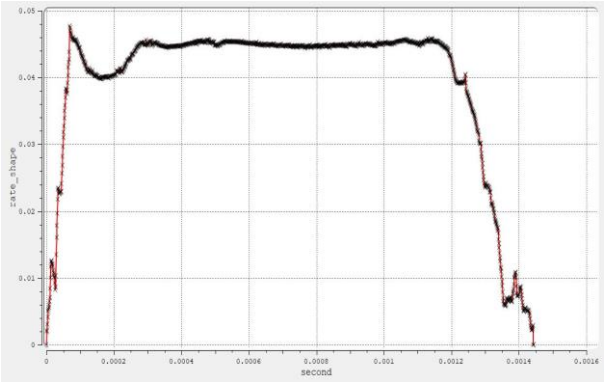

Figure 4. Injector rate shape v/s time(s)

Result and Discussion

To determine the ignition delay time, it is very crucial to define the SOI (start of injection) and SOC (start of combustion or Pressure Recovery Point). The SOI for all the simulations is set at 0ms and the SOC is defined as the time when the pressure in the chamber reaches 138KPa above the initial chamber pressure before the fuel injection [2]. The simulation was carried for 10ms with an initial time step of 1e-6s and a minimum timestep of 1e-8s. A SAGE detailed chemistry solver was used for the combustion modelling of both the surrogates. The various parameters like chamber pressure, Sauter mean diameter, spray tip penetration and vapor penetration were studied for all cases.

Chamber Pressure

The variation of chamber pressure with time for n-heptane can be seen in fig. 5. The curves clearly show an initial decrease in pressure due to the cooling effect of the liquid spray evaporation but then the chamber pressure suddenly increases because of heat release from chemical reactions. The pressure curve clearly distinguishes the physical and chemical ignition delay that can be seen by the sudden change in slope of the pressure curve at around 3ms. The total ignition delay (TID) of the fuel is the sum of physical ignition delay (PID) and chemical ignition delay (CID) [9]. The total ignition delay time for all the cases can be seen in table 1.

Sauter mean Diameter(SMD)

The variation of SMD with time for n-heptane can be seen in fig. 6. The curve shows that the SMD remains same in all the cases up to 3ms but an increase in the SMD with time can be seen at all the temperatures. A sudden increase in SMD was also observed during the time of autoignition.

Spray Tip Penetration

The spray penetration length was defined as distance from the nozzle tip to axial location of 95% of fuel mass fraction. The variation of spray tip penetration with time for n-heptane can be seen in fig. 7. The spray tip penetration is almost same for all the cases up to 1ms but after that point variation in spray tip penetration can be seen with maximum spray penetration of fuel found at chamber temperature of 770K. The spray tip penetration decreases with an increase in temperature and becomes completely zero at the time of autoignition.

Vapor Penetration Length

The vapor penetration length for all the cases can be seen in fig. 8. The vapor penetration length of the fuel is almost same at all the four temperatures and then immediately drops down to zero at the time of autoignition. The reason for fuel to show same behaviour in all cases up to 4ms is due to complete conversion of liquid phase of the fuel into vapor phase at such a high temperature.

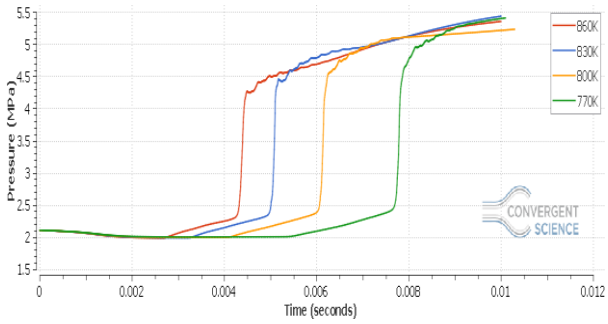

Figure 5. Variation of chamber pressure (MPa) with time(s) for n-heptane for four different chamber temperatures.

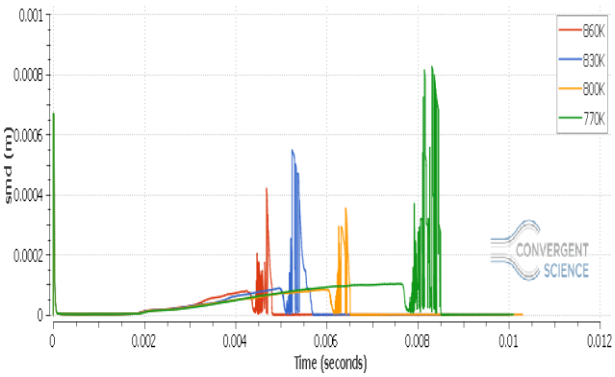

Figure 6. Variation in Sauter mean diameter(m) with time(s) for n-heptane for four different chamber temperatures.

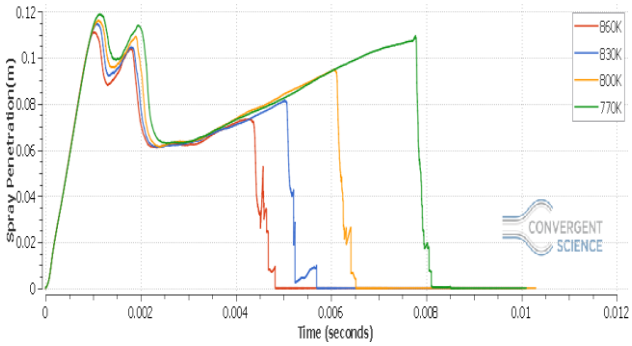

Figure 7. Variation of spray tip penetration(m) with time(s) for n-heptane for four different chamber temperatures.

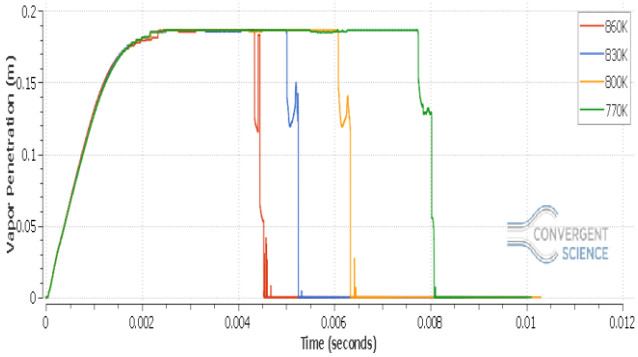

Figure 8. Variation in vapor penetration length(m) with time(s) for n-heptane for four different chamber temperatures.

S.no	Temperature(K)	TID for n-heptane (ms)	TID for multicomponent surrogate(ms)
1	770	6.58	6.32
2	800	5.28	5.10
3	830	4.34	4.12
4	860	3.71	3.47

Table 1. Total Ignition Delay for singlecomponent and multi component fuel surrogate for four different chamber temperatures.

Conclusions

A 3D model of high pressure and high temperature finite volume chamber was created to accurately and efficiently reproduce the ignition behaviour of single component and multi component surrogate of diesel fuel under different temperatures. The simulation was carried for a time interval of 10ms with an initial time step of 1e-6s and a minimum timestep of 1e-8s. The TID increases with the decrease in the chamber temperature. Also, the chamber temperature has more effect on the spray tip penetration over the vapor penetration. It was observed that the chamber pressure first decreases rapidly due to the evaporative cooling effect of liquid spray but then it increases as the chemical processes become dominant over the physical processes. During the time of autoignition, a rapid increase in chamber pressure and SMD was seen, but at the same time the spray and vapor penetration length becomes zero.

References

[1] Banish, G. Designing and Tuning High-Performance Fuel Injection Systems 2009, CarTech https://books.google.co.in/books?id=vmq7NiuaA78C

[2] G. E. Bogin Jr., A. DeFilippo, J. Y. Chen, G. Chin, Jon Luecke, M. A. Ratcliff, B. T. Zigler, and Anthony M. Dean. Numerical and Experimental Investigation of *n*-Heptane Autoignition in the Ignition Quality Tester (IQT). *Energy Fuels*, 2011, *25* (12), pp 5562–5572. October 13, 2011. DOI**:** 10.1021/ef201079g

[3] J. Bacha, J. Freel, A. Gibbs, L. Gibbs, G. Hemighous, K. Hoekman, J. Horn, M. Ingham, L. Jossens, D. Kohler, D. Lesnini, J. McGeehan, M. Nikanjam, E. Olsen, R. Organ, B. Scott, M. Sztenderowicz, A. Tiedemann, C. Walker, J. Lind, J. Jones, D. Scott and J. Mills, *Diesel Fuels Technical Review*, Chevron Products Company, 2007

[4] K. huber, J. Hauber "Engine bases test method for determining the ignition quality of diesel fuels" MTZ Motortechnische Zeitschrift 74(11):904-911 DOI: 10.1007/s35146-013-0266-4

[5] Liu, A., Mather, D., and Reitz, R., "Modelling the Effects of Drop Drag and Breakup on Fuel Sprays," SAE Technical Paper 930072, 1993, https://doi.org/10.4271/930072.

[6] Mubarak Ali, M., Elhagrasy, A., Sarathy, M., Chung, S. et al., "Auto-Ignition and Spray Characteristics of n-Heptane and iso-Octane Fuels in Ignition Quality Tester," SAE Technical Paper 2018-01-0299, 2018, https://doi.org/10.4271/2018-01-0299.

[7] Naser N, Yang SY, Kalghatgi G, Chung SH. Relating the octane numbers of fuels to ignition delay times measured in an ignition quality tester (IQT). Fuel 2017; 187:117–27. https://doi.org/10.1016/j.fuel.2016.09.013

[8] Xiuxiu Sun, Xingyu Liang, Hanzhengnan Yu, Yajun Wang, Zhijie Zhu "Comparison the Performance of N-heptane, N-dodecane, N-tetradecane and N-hexadecane" May 2017 Energy Procedia 105:1426-1433 DOI: 10.1016/j.egypro.2017.03.533

[9] Z. Zheng, T. Badawy, N. Henein, E. Sattler, "Investigation of physical and chemical delay periods of different fuels in the ignition quality tester," J. Eng. Gas Turb. Power 135 (2013) 061501.