Simulation of the ignition mechanisms of low and high octane number blended fuels in HCCI engine

IOP Conf. Series: Materials Science and Engineering **788** (2020) 012058 doi:10.1088/1757-899X/788/1/012058

Simulation of the ignition mechanisms of low and high octane number blended fuels in HCCI engine

Munthanna Jamil[1,*], Mohd Adnin Hamidi[1] Ahmad Fitri Yusop[1], Muhammad Anas Abdul Aziz[1], Mohamad Fathin Hamidi[1], Tatchineswaranpillai Sundram[1]

[1] Faculty of Mechanical Engineering, Universiti Malaysia Pahang, 26600 Pekan, Pahang, Malaysia

*Corresponding author: muthannajamil@gmail.com

Abstract. Homogenous Charge Compression Ignition (HCCI) is an alternative combustion concept for in reciprocating engines which offers significant benefits in terms of its high efficiency and low emissions. HCCI is the most commonly used name for the auto-ignition of various fuels and one of the most promising alternatives to SI and CI combustion. This study focus on the ignition reactions of low and high octane number of fuel blends through comprehensive simulation. This study was carried out by using n-heptane as a base fuel and toluene as a sub fuel use as a fuel mixture in this simulation. Furthermore, for numerical analysis, MATLAB Software has been used to design simplified model of reaction mechanism for n-heptane. The simplified model has been discussed in this study. The highest value of hydroxyl radicals OH was achieved at approximately 0.23 at NTF 10 (Toluene mixture 10%) and the line decreased until 0 This value is gradually decreased when the mixture of toluene (NTF) as sub fuel is elevated until NTF60 Due to the content percentage of toluene added 10% consecutively, HCHO production increased as well. It is because HCHO consumes OH and at the same time affects the amount of OH. By doing this method (mixing n-heptane with toluene), the ignition delay of the fuel becomes longer is described. It is also shows that the simplified model constructed with a consideration of the property of reaction happen in n-heptane (base fuel) added with toluene (sub fuel) in which OH reproduction and fuel + OH reaction plays important role. The purpose of this study is to figure out the reaction mechanism of compression ignition at Low Temperature Oxidation (LTO) and design the simplified model of reaction mechanism for n-heptane + toluene (NTF).

Keywords. Low temperature oxidation; Homogenous Charge Compression Ignition (HCCI); Toluene; n-heptane; Graphical User Interface (GUI)

1. Introduction

Nowadays, we see that hydrocarbon fuels are an essential source of energy used for transportation in our daily life. The combustion models for these fuels are used to predict the performance of internal combustion engines. With these combustion models, engines can be designed to improved efficiency and reduced emissions in system. Combustion, also known as burning, is the basic chemical process of releasing energy from a fuel and air mixture. In an internal combustion engine, the ignition and

combustion of the fuel occurs within the engine itself. The internal combustion engine is an engine that uses the explosive combustion of fuel to push or move a piston within the cylinder engine [1].

Homogeneous Charge Compression Ignition (HCCI) engine is a promising alternative with high thermal efficiency and ultra-low emission characteristics to the existing internal combustion engines. HCCI combustion is the process in which a homogeneous mixture is auto-ignited through compression. HCCI has the potential to reduce both particulate matter and NO_x emissions while maintaining the fuel efficiency [2]. Recent research has shown that the use of two fuels with different reactivity (such as gasoline and diesel) can help solve some of the difficulties of controlling HCCI ignition and burn rates [3]. RCCI or Reactivity Controlled Compression Ignition has been demonstrated to provide highly efficient, low emissions operation over wide load and speed ranges [4, 5].

The oxidation of normal n-heptane (nC_7H_{16}) already has been subject of many experiments and model of the studies. But still most of the studies were carried out under High Temperature Oxidation (HTO) and very few to the Low Temperature Oxidation (LTO) of the n-heptane especially regarding the characterization reaction products [6]. Low temperature oxidation (LTO) of hydrocarbons is of importance for the development of diesel and homogenous charge compression ignition (HCCI) engines, as this particular chemistry triggers auto-ignition phenomena. Low Temperature Oxidation is a reaction which occurs at or below room temperature (usually 500K-1000K). The first modelling studies of the oxidation of n-heptane were carried out in the late of 1970s and in the 1980s by Coats and Williams where only for high temperature oxidation [6, 7]. In 1989, Westbrook has proposed the first detailed kinetic accounting for the low and high temperature oxidation of n-heptane [8, 9]. Since then, several of low and high temperature of this species has been introduced.

This study objectives focuses on ignition mechanism's reaction of compression ignition at Low Temperature Oxidation (LTO) by develop the simplified model of reaction mechanism of fuel mixture, and numerical simulation by using MATLAB software where the ignition behaviour of n-heptane changing with the fuel mixing ratio. Recently, many research focused on simplified model of PRF [10-13], with most of them concentrating on experiment of ignition timing or high-temperature oxidation reaction, but less in the low-temperature oxidation reaction. Because of that, in this study we tried to focus on middle product from low-temperature oxidation and bring reaction mechanism. Low temperature oxidation (LTO) of hydrocarbons is of importance for the development of diesel and homogenous charge compression ignition (HCCI) engines, as this particular chemistry triggers auto-ignition phenomena. A Low Temperature Oxidation (LTO) region is highly depending on complicated chemical reaction mechanism as well as ignition delay and also for reaction pathway of both base fuel and sub fuel. In this project, by developing a simplified model of the reaction mechanism of fuel mixture (base fuel and sub fuel), the analysis of the reaction mechanism of the fuel mixture in low temperature oxidation becomes easier in term of time effective because it can minimize the time by doing this concept of analysis.

There are two-stage of heat generation from ignition mechanism of hydrocarbons. Relatively, around 700K there is small heat generation called "Cool Ignition" while around 1000K, there is a large heat generation as main combustion flame called "Hot Ignition". This Hot ignition is dominated and influenced by the Cool Ignition. This phenomenon is showed in figure 1.

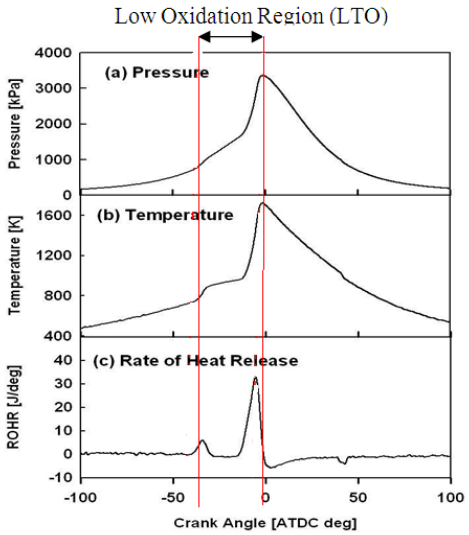


Figure 1. Observed pressure (a), temperature (b) and rate of heat release (c) in n-heptane fueled HCCI engine.(φ= 0.43, intake gas temperature = 413K) [15].

Heat generation for low temperature oxidation and thermal ignition preparation period has significant influence to the time when the temperature reached for the occurrence of hot flame. In addition, by supplying OH reactant into H_2O_2 presence reaction can accelerate the generation of hot flame. Therefore, to understand and control low temperature oxidation reaction that has dominated cool flame that cause the hot flame as the main combustion becoming important task in realizing HCC1 engine. Figure 2 shows schematic diagram of the low temperature oxidation reaction in hydrocarbon fuel [6].

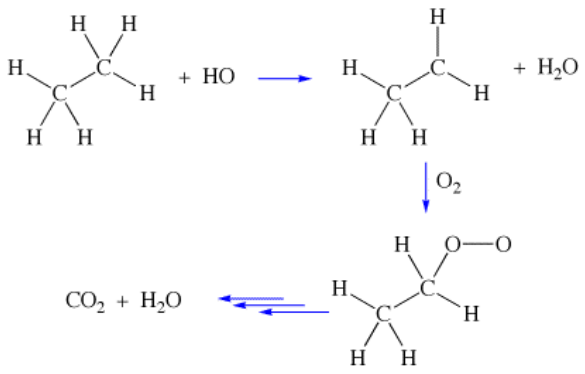


Figure 2. General Oxidation Scheme for hydrocarbon [15].

For the numerical simulation, it use the MATLAB software for the numerical analysis which by creating the Graphical User Interface (GUI) using this software. The design GUI simulation program consist of assumed parameters input, calculation output and data calculation.

2. Methodology

In the present study, the simulation models were compared or validated by the experimental results that were conducted on a four stroke single cylinder diesel engine (displacement 541 cm3,

compression ratio 18.0) which was maintained the standard speed at 600 RPM and externally driven by an electric motor for constant speed operation regardless of internal power generation [6]. The methodology of this study been constructed from two main process. First, are the modelling process and the numerical procedure by using the MATLAB Software. A simplified model will be created in translated to MATLAB Software. In MATLAB Software, GUI methods will be used. After run the simulation the result will be translated into summary graph than can be plotted in Excel file. All results from executed simulation will be translated to compare with experimental result obtained from Adnin et al. [6] because this study using the same fuels and parameters in the simulation model.

For PRF and NTF, iso-octane and toluene was selected. Within PRF fuel, iso-octane (1. $iC_{g)}$ and Toluene (1.C_6H_6C) has high knocking resistance with octane number 100 and 110 respectively, while n-heptane (1.nC_7h) with low knocking resistance has 0 octane number. Toluene is a typical high octane number fuels that reduce ignition activity of n-heptane when mixed, but some different behaviours between these fuels on the ignition control [14].

The design GUI simulation program consist of assumed parameters input, calculation output and data calculation. The simulation is run by different percentage of NTF. NTF is the fuel with a mixture of toluene and n-heptane. First, to start the simulation, run the program and setup the parameters by input the value of initial condition of each parameter. Then, the program will stimulate the calculation of the modelled evolution of chemical composition in Low Temperature Oxidation (LTO) and the result will be displayed in a graph.

2.1 Discussion with simplified model

The low temperature oxidation mechanism of hydrocarbons consists of complicated reactions such as H-abstraction, O2-addition, isomerization, second O2-addition, decomposition and branching passes. The oxidation mechanism of mixture of n-heptane (base fuel) and iso-octane or toluene (second fuel) is expressed in a summarized manner as below;

$$nC7H16+OH \rightarrow \alpha bOH+ \beta bHCHO+other\ products \quad (1)$$

$$iC8H18\ (or\ C6H5CH3)+OH \rightarrow \alpha sOH+ \beta sHCHO+other\ product \quad (2)$$

Where $\alpha b,s$ can be expressed as the reproduction index of OH from base or second fuel, and $\beta b,s$, the reproduction yield of chain terminating intermediate represented by HCHO from base or second fuel. Other products are represented as an unreactive during the course of low temperature reaction.. Differential equations time evolution of relevant species can be described as;

$$d[nC7H16]dt=-kb[C7H16][OH] \quad (3)$$

$$d[subfuel]dt=-ks[subfuel][OH] \quad (4)$$

$$d[OH]\quad dt=\{(\alpha b-1)kb[C7H16]+(\alpha s-1)ks[subfuel]-ka[HCHO]\}[OH] \quad (5)$$

$$d[HCHO]dt=\{\beta bkb[C7H16]+\beta sks[subfuel]-ka[HCHO]\}[OH] \quad (6)$$

From the equation (3) until (6), where *kb,s* is the rate constant of base or second fuel with OH product, and α expressed as a aldehyde. From the equation, it can be translated into a form in which the independent variable which is percentage consumption of base fuel, known as *x*, which are below [6]:

$$dys=-(g1ys1-x)dx \quad (7)$$

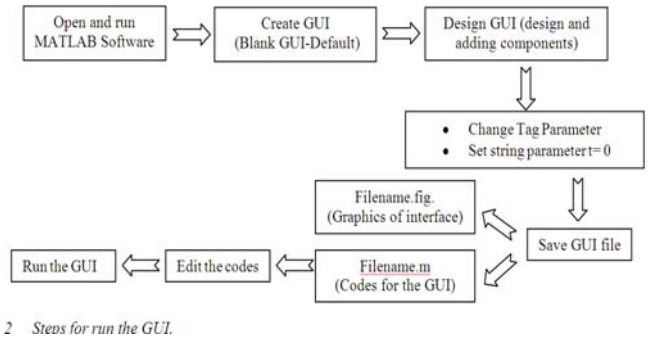
$$dyald=(\beta b-\beta sys1-x-g21-x)dx \quad (8)$$

$$dyOH=((\alpha b-1)+(\alpha s-1)g1ys1-x-g2yald1-x)dx \quad (9)$$

From the previous equation, *ys* is the remaining amount of second fuel (relative to initial amount of base fuel and so forth), *yald* is the accumulated amount of aldehyde, and *yOH* is the amount of OH product, $g1= ks/kb$ and $g2= ka/kb$, where $g1$ is the ratio of rate constant between second fuel with OH and base fuel with OH, and $g2$ is the ration of rate constant between aldehyde with OH and base fuel with OH. The αb of low octane number of fuel is necessarily exceeding unity, but αs may differ. The OH concentration increases with repetition of the reaction chain when initial overall OH reproduction index is over unity. The slope of OH increase gradually reduces and finally the chain system is terminated that according to decrease in fuel and increase in the OH consuming aldehyde. The point of termination is represented by the overall OH reproduction index = 1 [6]. The parameters used for NTF (n-heptane and toluene mixture) are $kbks$=5, αb=2, αs=0, βb=1.6, and βs=0. It is a part of which was assumed by overlooking the toluene oxidation mechanism [12].

2.2 Basic steps for numerical procedure

2.1.1. Creating Graphical User Interface (GUI). Figure 3 shows the steps for run the GUI.

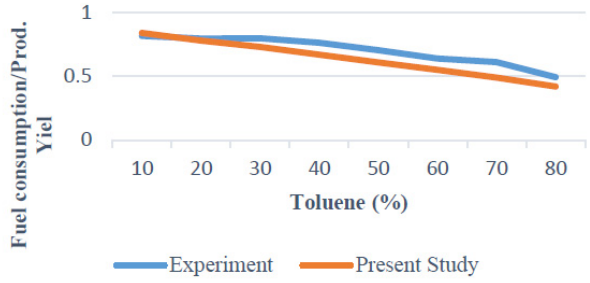


2 Steps for run the GUI.

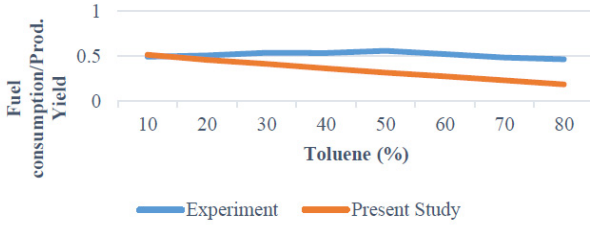
Figure 3. Steps for run the GUI.

2.1.2. Validation. To further validate the applicability of the developed reaction mechanism for auto-ignition combustion, numerical simulations were performed and compared against the HCCI engine experiments. The numerical simulation was able to capture elements of HCCI combustion of n-heptane and toluene mixture fuel, particularly the LTO.

In addition, figure 4 shows that the total comparison of results between the model calculation, simulation (CHEMKIN) experimental and GUI result for validation purposes Meanwhile for validation with Adnin et al experimental result, the n-heptane and toluene consumption been compared as shows in figure 4. The figure show the margin error is below 9% for n-heptane consumption and 15% for toluene consumption.



a) N-heptane consumption



b) Toluene consumption

Figure 4. Comparison between simplified model with experimental results.

It is shows that the simplified results for toluene and n-heptane patterns are similar to GUI results. There are differences because of the parameters that been considered are different. It is because the GUI results are focusing on the LTO which a lot of parameters or condition doesn't have much impact on that situation.

Statistical analysis is conducted to study the variability and stability of raw data. The margin error between the simulation data and experimental result is below 5% during validation. Muthanna in [16] mentioned that 30 data points could gain 18 degrees of freedom and 16.7% uncertainty for checking the capability of the process. It is based on the Wheeler's Graph (2004).

3. Results and discussion

The aim of this study is focuses on ignition mechanism's reaction at Low Temperature Oxidation (LTO) by using simulation modelling and numerical simulation. The result of this simplified model is plotted into "Fraction to Initial n-heptane" versus "n-heptane Consumption x" and also all results will be summarised in one graph (figure 5).

These calculations show that the toluene consumption (*yt)* is less than n-heptane consumption, the effect of reducing n-heptane consumption is less than in toluene, and aldehyde production (*yald*) increases with decreasing toluene content. Interaction between the mixture of fuel components (n-heptane + toluene) will be resulting decrease in n-heptane consumption because of competition between n-heptane with OH and toluene with OH reaction rate. Toluene is typical high octane number fuels that reduce the ignition activity of n-heptane when mixed [15].

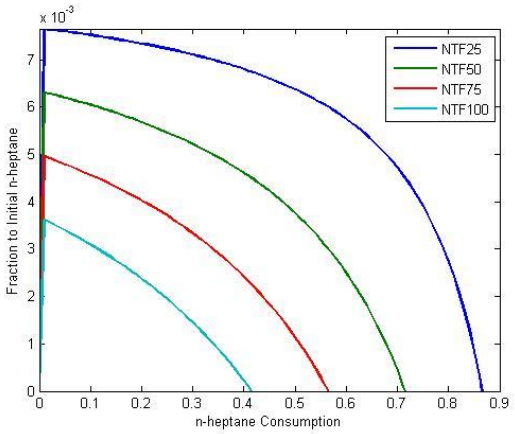


Fig. 5. Comparison in final composition of OH in LTO from various percentages of NTF.

Figure 5 shows a comparison of OH production graph for NTF fuels from a different percentage of toluene. From the graph, it can be observed that by increasing toluene percentage, OH production become decrease as predicted by toluene character. Adnin et al. in [15] mentioned that OH as the middle product that propagates high temperature oxidation decrease by increasing toluene percentage.

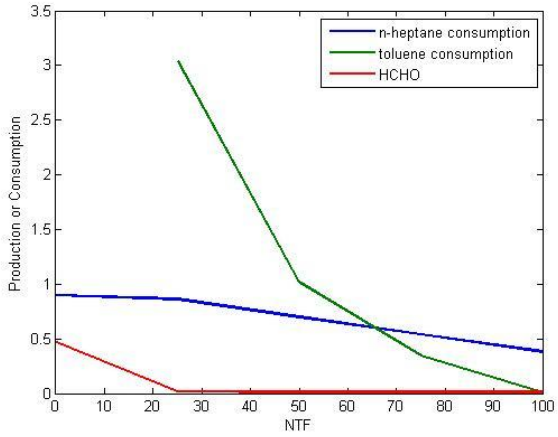


Figure 6. Fuel consumption and formaldehyde production at the end of low temperature chain reaction in NTF.

From figure 6, it shows that the high percentage of toluene, the chain reaction does not start from the beginning, so that low temperature oxidation (LTO) heat release does not occur. To summarize the mixing effect of high octane number of fuel to n-heptane ignition property, toluene acts as a simple dilution agent, since the toluene-OH reaction rate is slow and OH production index is very low as mentioned by Adnin et al in [15]. Fuel consumption decreases with increasing of toluene/n-heptane ratio although it is weak. It is because toluene has lower rate constant with OH, so that toluene barely interrupts the OH reproducing chain reaction of n-heptane as stated by Adnin et al in [15]. The reaction mechanism is quietly complicated but already been approved through many research. In the previous study, there are a 26 reactions and 25 species mechanism for n-heptane which has been derived from two detailed mechanisms for developed by Lawrence Livermore National Laboratory (LLNL) mentioned by Adnin et al in [15]. Figure 7 are the results from [15] shows the comparison

between CHEMKIN and experimental result run by Adnin et al. Meanwhile figure 8 shows the other results that compares between simpolified model calculation and CHEMKIN result based on [15] parameters.

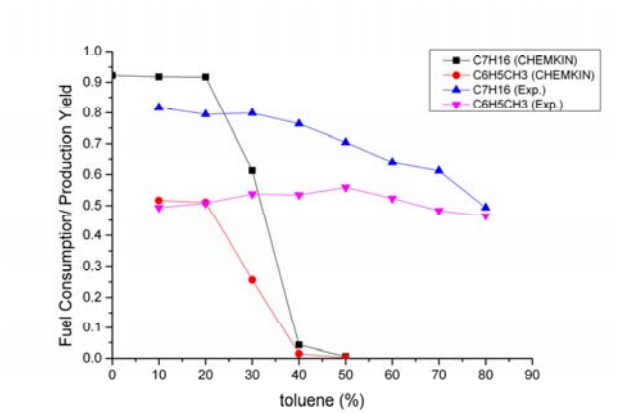


Figure 7. Graph comparison between simulation (CHEMKIN) and experimental results [15].

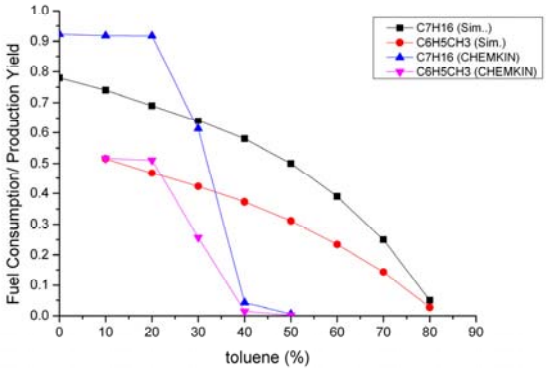
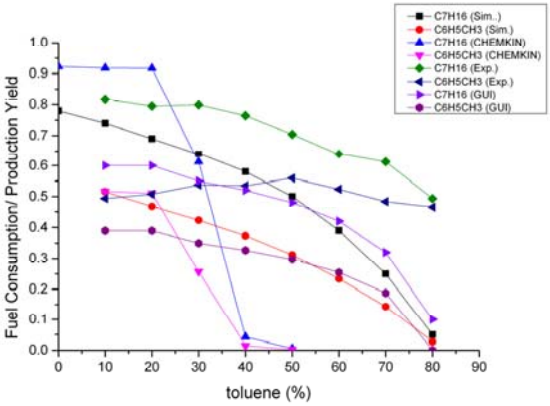


Figure 8. Graph comparison between simplified model calculation and simulation (CHEMKIN).



[15]

Figure 9. Graph comparison between model calculation, simulation (CHEMKIN), experimental and GUI results.

In figure 9, it shows the comparison between result in [15] (CHEMKIN, Simplified Model and Experimental) with GUI results. Graph shows the GUI pattern is more similar to the experimental result compare to CHEMKIN and it's expected because CHEMKIN input of parameter and consideration is greater than the GUI.

4. Conclusion

From the result simulation, it can be concluded that the amount of toluene content becomes decreasing with the increasing of n-heptane consumption, and the aldehyde production also increases with the decreasing of toluene content. Moreover, the increasing of toluene percentage has big influence in OH production. It is because OH production becomes decrease as predicted by toluene character and OH as the middle product that propagates high temperature oxidation decrease by increasing toluene percentage. It also can be concluded that the GUI can be use as a tools for describing the ignition mechanism's reaction at LTO but more parameter settings required for more precise results.

In the future works, there are some improvements need to be considered in order to ensure the success of this project with less errors during simulation. During setup the parameters of this program simulation, there is some calculation errors that have been shown in the graph. In order to solve this problem, to learn more about MATLAB software such as loop calculation, MATLAB Simulink or other software which can calculate based on the simplified model equations. Other than that, for further research, we can consider other parameters such as temperature and pressure in the model calculation to improve the data calculation. Also, it can be referenced for comparison between fuel combustion simulation and fuel combustion experiment.

Acknowledgement

The authors are grateful to the Universiti Malaysia Pahang (UMP) for financial supports given under research grand scheme RDU190358

References

[1] R. Ferguson and A. T. Kirkpatrick 2015, *Internal combustion engines: applied thermosciences*: John Wiley & Sons.

[2] F. Zhao, T. W. Asmus, D. N. Assanis, J. E. Dec, J. A. Eng, and P. M. Najt, 2003 "Homogeneous charge compression ignition (HCCI) engines: key research and development issues PT-94," *Progress in technology,* vol. 94.

[3] M. Yao, Z. Zheng, and H. Liu 2009, "Progress and recent trends in homogeneous charge compression ignition (HCCI) engines," *Progress in Energy and Combustion Science,* vol. 35, pp. 398-437.

[4] R. D. Reitz and G. Duraisamy 2015, "Review of high efficiency and clean reactivity controlled compression ignition (RCCI) combustion in internal combustion engines," *Progress in Energy and Combustion Science,* vol. 46, pp. 12-71.

[5] S. L. Kokjohn, R. M. Hanson, D. Splitter, and R. Reitz 2011, "Fuel reactivity controlled compression ignition (RCCI): a pathway to controlled high-efficiency clean combustion," *International Journal of Engine Research,* vol. 12, pp. 209-226.

[6] M. A. B. Hamidi 2016, "Ignition Mechanism Analyzed through Transient Species Measurements and its Correlation with 0-D and 3-D Simulations for PRF and Toluene/n-Heptane Mixture,".

[7] C. Coats and A. Williams 1979, "Investigation of the ignition and combustion of n-heptane-oxygen mixtures," in *Symposium (International) on Combustion*, pp. 611-621.

[8] C. K. Westbrook and F. L. Dryer 1984, "Chemical kinetic modeling of hydrocarbon combustion," *Progress in Energy and Combustion Science,* vol. 10, pp. 1-57.

[9] C. Westbrook, "J. r. Warnatz and WJ Pitz 1989, A Detailed Chemical Kinetic Reaction Mechanism for the Oxidation of Iso-Octane and n-Heptane over an Extended Temperature Range and its Application to Analysis of Engine Knock," in *Twenty-Second Symposium*

(International) on Combustion, The Combustion Institute, pp. 893-901. 32
[10] C.K. Westbrook, F.L. Dryer 1984, Prog. Energy Combust. 10 (1) 1–57.
[11] C.K. Westbrook, J. Warnatz, W.J. Pitz 1989, Symp. (Int.) Combust. 22 (1) 893–901.
[12] E. Ranzi, P. Gaffuri, T. Faravelli, P. Dagaut, 1995, Combust. Flame 103 (1–2)91–106.
[13] R.P. Lindstedt, L.Q. Maurice 1996, Combust. Sci. Technol. 120 (1–6) 119–167.
[14] G. Shibata and T. Urushihara 2008, "Dual phase high temperature heat release combustion," *SAE International Journal of Engines,* vol. 1, pp. 1-12.
[15] M. A. B. Hamidi, 2016, Ignition Mechanism Analyzed through Transient Species Measurements and its Correlation with 0-D and 3-D Simulations for PRF and Toluene/ n-Heptane Mixture. University Toyama, Toyama, Japan.
[16] Muthanna,Jamil and Noraini,Mohd Razali 2016 *Simulation of Assembly Line Balancing in Automotive Component Manufacturing*. In: IOP Conference Series: Materials Science and Engineering: 2nd International Manufacturing Engineering Conference and 3rd Asia-Pacific Conference on Manufacturing Systems (iMEC-APCOMS 2015), 12–14 November 2015 , Kuala Lumpur, Malaysia. pp. 1-8., 114 (1). ISSN 1757-8981 (Print); 1757-899X
[17] J. E. Witzky and J. J. M. Clark 1964, "Stratified spark ignition internal combustion engine," ed: Google Patents.
[18] A. Tezaki, T. Miyashita, And H. Murasawa 2008, "HC3-4: Transient Chemical Composition Analysis in HCCI of n-Heptane Fuel (HC: HCCI Combustion, General Session Papers)," in *TheProceedings of the International symposium on diagnostics and modeling of combustion in internal combustion engines 2008.7*, pp. 329.
[19] D. Gentile 2017, "External combustion engine," ed: Google Patents.
[20] W. P. Willard 2004, "Engineering fundamentals of the internal combustion engine," *Editorial Prentice Hall. New Jersey*.
[21] V. Ganesan 2012, *Internal combustion engines*: McGraw Hill Education (India) Pvt Ltd.
[22] H. Zhao 2007, HCCI and CAI engines for the automotive industry: Elsevier.
[23] X.-c. Lü, W. Chen, and Z. Huang 2005, "A fundamental study on the control of the HCCI combustion and emissions by fuel design concept combined with controllable EGR. Part 1. The basic characteristics of HCCI combustion," *Fuel,* vol. 84, pp. 1074-1083.
[24] R. K. Maurya and A. K. Agarwal 2011, "Experimental study of combustion and emission characteristics of ethanol fuelled port injected homogeneous charge compression ignition (HCCI) combustion engine," *Applied Energy,* vol. 88, pp. 1169-1180.
[25] R. H. Stanglmaier and C. E. Roberts 1999, "Homogeneous charge compression ignition (HCCI): benefits, compromises, and future engine applications," SAE Technical Paper 0148-7191.
[26] K. Epping, S. Aceves, R. Bechtold, and J. E. Dec 2002, "The potential of HCCI combustion for high efficiency and low emissions," SAE Technical Paper