

A NUMERICAL STUDY OF GASOLINE SURROGATE COMBUSTION ON HOMOGENEOUS CHARGE COMPRESSION IGNITION ENGINES

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Abstract. In this work, a numerical study of gasoline surrogate combustion on engine-like conditions was performed. The engine was numerically represented as a Homogeneous Charge Compression Ignition engine. One detailed multicomponent kinetics model for gasoline surrogates available at literature was used in order to analyze the ignition-based combustion on the engine. Two fuels surrogate formulations were used in this work; FS#1((i-octane/toluene/n-heptane/di-iso-butylene/ethanol, 30%/25%/22%/13%/10% vol.) and FS#2 (toluene/i-octane/n-heptane/di-iso-butylene 45%/25%/20%/10% vol.). Information about pressure, temperature, heat release and chemical species formation/depletion were obtained as function of crankshaft rotation during the compression and combustion/expansion strokes in the internal combustion engine. Three stoichiometric mixture compositions were tested covering rich and lean engine operation conditions. The study was carried out using the HCCI (homogeneous charged compression ignition) model in the CHEMKIN software. The numerical simulations shows different compression-ignition based behaviors for FS#1 and FS#2, as function of the difference of the volumetric compositions.

Keywords: HCCI, Internal combustion engines, gasoline surrogate

1. INTRODUCTION

Autoignition is a critical parameter of study in internal combustion (IC) engines, since it causes knock, which limits efficiency and causes structural damages, in spark ignition (SI) engines and is the mechanism by which heat release occurs in compression ignition (CI) and homogeneous charge compression ignition (HCCI) engines. Figure 1(adapted from Heywood, 1988) shows three situation of engine operations, the first one (a) at normal combustion behavior where the engine is operating at the projected operation pressure.

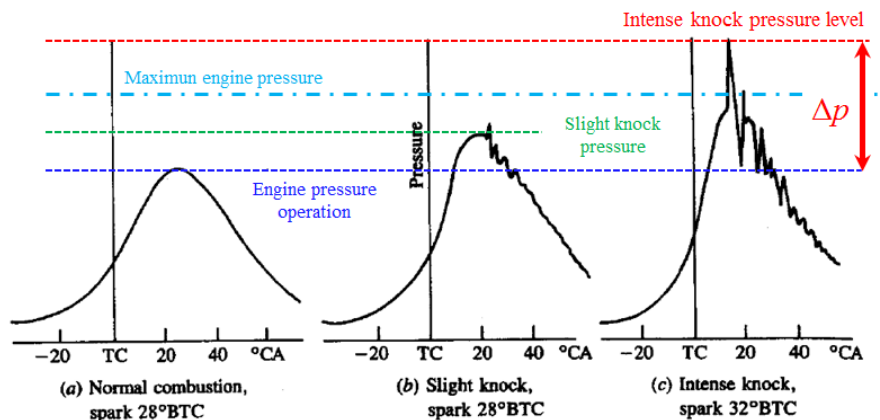


Figure 1. Normal combustion, slight knock and intense knock behaviors in internal combustion engines (Adapted from Heywood, 1988)

In the second situation, the pressure is higher than the projected operation pressure of the engine, but still below the critical value defined by the structural design of the engine. In the third situation, the engine is operating under very critical detonation conditions, the pressure is higher than the maximum value defined by the structural design of the engine, at this point and after some combustion cycles very seriously damages can release in the engine, as showed on Figure 2. It is clear that the situation (c) on Figure 1 is the result of the increase of 4° in the sparking time for the sparking release, 28° before the top dead center on situations (a) e (b) and 32° before the top dead center on situation (c). However, this same behavior (knocking) may be the result of one of two factors: i) fuel pre-ignition by hot surfaces or ii) autoignition of the mixture. Several research groups have been developing research on understanding the causes of fuel pre-ignition by hot surfaces, Suga et al. (1989) examined the pre-ignition methanol (M85) using the technique of post-ignition using a 4-valve engine with a fixed compression ratio of 10.8, and three rotational speeds, using a heated surface emulating a hotspot within the combustion chamber. Menrad et al. (1982) analyzed the pre-ignition combustion of alcohols at high values of compression ratio using two internal combustion engines with different compression ratio, various operating parameters were analyzed for the occurrence of detonation in order to

correlate physical properties of fuels analyzed. Hamilton et al. (2008) analyzed the characteristics of pre-ignition of ethanol and gasoline / ethanol (E85) in internal combustion engine CFR spark ignition, using a glow plug (Diesel glow plug type) to induce pre-ignition, emulating a hot spot (hot surface) in the combustion chamber. Mendirata and Pundir (1993) analyzed the pre-ignition of fuels with high content of olefins in an internal combustion engine spark ignition and a couple of times. The choice of two-stroke engine is influenced mainly by lubricating oil that has in the combustion process in such engines.



Figure 2. Damages in internal combustion engines caused by operating on knocking regime

Conversely at literature can be found a considerable number of research papers on autoignition of hydrocarbon mixtures, most of them pure fuels and mixtures up to four compounds and just one research work for mixtures with five compounds.

The purpose of this work is to understand the numerical response of the available detailed kinetics models for gasoline surrogates under engine like conditions by using two different gasoline surrogate formulations.

2. DETAILED KINETICS MODEL

Detailed kinetics models for multicomponent gasoline surrogates are scarce at literature. Kinetics models for pure fuels and blend of pure fuels up to three compounds is a little easier to found. At literature, it can be found only one detailed kinetics model for quinary mixtures completely validated against experimental results of pure and blends of compounds (up to five compounds). In this work, was used the quinary gasoline surrogate mechanism developed by Cancino et al. (Cancino et al., 2011). The mechanism was obtained merging existing chemical kinetics substructures which modeled the species that composed the surrogate mixture.

The composition of the surrogate was chosen according to five species which chemically represented the main classes of hydrocarbons in gasoline. The initial kinetics model was the PFR (Primary Reference Fuels, composed by iso-octane and n-heptane) model of Curran et al (1998). The ethanol oxidation kinetics were added from (Cancino et al., 2009a) and (Cancino et al., 2009b), which was the mechanism of Marinov (1999) improved using Konnov's mechanism (2000). The resulting mechanism was combined with the toluene sub-mechanisms of Andrae et al. (2007) and Maurice (1996), and the diisobutylene sub-kinetics of Metcalfe et al. (2007). The resultant mechanism for a multicomponent ethanol-based gasoline surrogates consists of 1130 chemical species among 5242 elementary reactions.

3. HOMOGENEOUS CHARGE COMPRESSION IGNITION MODEL

3.1 Model description

The HCCI model simulates the combustion process on internal combustion engine under auto-ignition conditions, most relevant to the study of fuel auto-ignition behavior, engine knock, and homogeneous charge compression ignition (HCCI) engines. In order to better understand the model, it is necessary to explain the geometric parameters involved. Figure 3, shows the main parameters defining the geometry of a reciprocating engine.

From Figure 3, can be developed several relationships, as done by Heywood, 1988, as follows:
Compression ratio:

$$r_c = \frac{V_d + V_c}{V_c} \quad (1)$$

Ratio of connecting rod to crank-arm radius:

$$R_{bs} = \frac{B}{L} \quad (2)$$

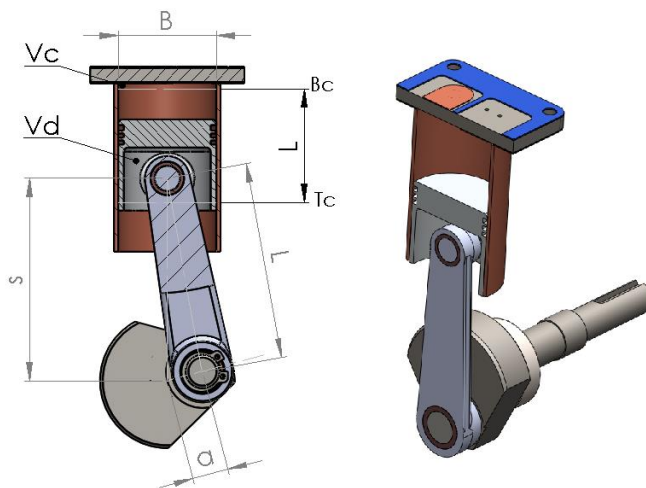


Figure 3. Basic geometry of a reciprocating engine (adapted from Heywood, 1988)

Distance between the crankshaft axis and the piston pin axis:

$$s = a \cos \theta + (l^2 - a^2 \sin^2 \theta)^{1/2} \quad (3)$$

Ratio of total volume to clearance volume (combustion chamber volume):

$$\frac{V}{V_c} = 1 + \frac{1}{2}(r_c - 1) \left[R + 1 - \cos \theta - (R^2 - \sin^2 \theta)^{1/2} \right] \quad (4)$$

The software CHEMKIN simulates the kinetics process as a variable-volume reactor, assuming isentropic compression, for every step or rotation of the crankshaft (θ). After every step of crankshaft rotation, the pressure is calculated by assuming isentropic compression as follow:

$$\frac{P_{motored}}{P} = \left(\frac{V}{V_{ref}} \right)^\gamma \quad (5)$$

where γ is the specific heat ratio. For every calculated volume and pressure values after the crankshaft step rotation, the CHEMKIN software uses the mass, energy and species conservation equations in order to estimate the temperature and chemical species distribution.

3.2 Numerical conditions for simulations

Table 1 shows the composition of the fuels surrogates used in this work and engine operating conditions. Three stoichiometries ($\Phi = 1.1, 0.5$ and 0.25) covering lean and rich mixtures.

The volume of the combustion chamber was kept constant as well as the crankshaft rotation velocity and intake pressure. In function of the of octane number differences between the fuels surrogates, it was necessary to test both the mixtures at different compression ratio and intake temperature mixture. The RON/MON numbers of FS#1 and FS#2 are 95.1/86.7 and 94.6/85 respectively.

Table 1. Fuel surrogates composition and engine operating conditions

Mixture	Fuel Surrogate #1	Fuel Surrogate # 2
Ethanol (% vol)	10	---
i-Octane (% vol)	30	25
n-Heptane (% vol)	22	20
Di-iso-butylene (% vol)	13	10
Toluene (% vol)	25	45
Engine Conditions		
Compression ratio	8.9	10
Combustion chamber volume (cm ³)	150	150
Engine connecting Rod to Crank Radius Ratio	3.71	3.71
Engine Speed (rpm)	2200	2200
Initial Temperature (K)	447	600
Intake pressure (atm)	1.065	1.065

4. NUMERICAL RESULTS

Two gasoline surrogates pursuing different composition and octane numbers were tested under engine like conditions. Table 1 shows the volumetric compositions and engine operating conditions.

4.1 Fuel surrogate #1 (i-octane/toluene/n-heptane/di-iso-butylene/ethanol, 30%/25%/22%/13%/10% vol.)

Figure 4 shows the numerical results of pressure and temperature as function of the crankshaft position. It can be observed that for rich conditions the maximum temperature value is higher when compared to lean mixtures, indicating that the detailed kinetics model is thermodynamically consistent. Also, Figure 4 shows that the maximum peak of pressure is moving to the left side of the figure as stoichiometry is decreasing.

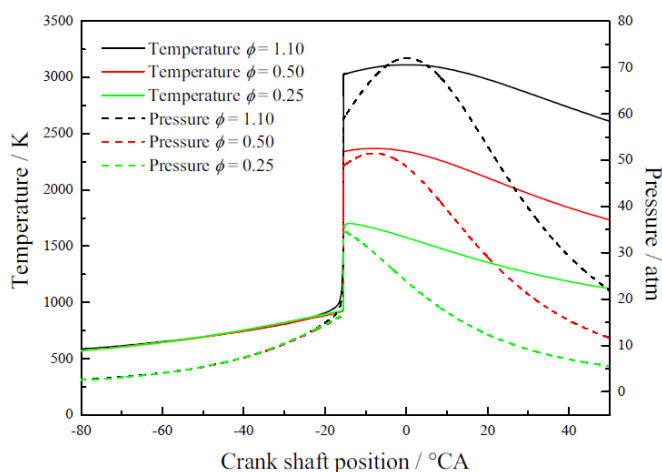


Figure 4. Temperature and pressure as function of the crankshaft position – results for gasoline surrogate #1

It was not observed big differences of the crankshaft position for maximum heat release in function of the stoichiometry. The results of Figure 4 are in completely agreement with the results on Figure 5, this figure shows the heat release and chemical species in function of the crankshaft position in the region very near to the maximum heat release (15.45° before the top dead center). It can be observed that rich mixtures start before the heat release and radical species formation when compared to the lean mixture.

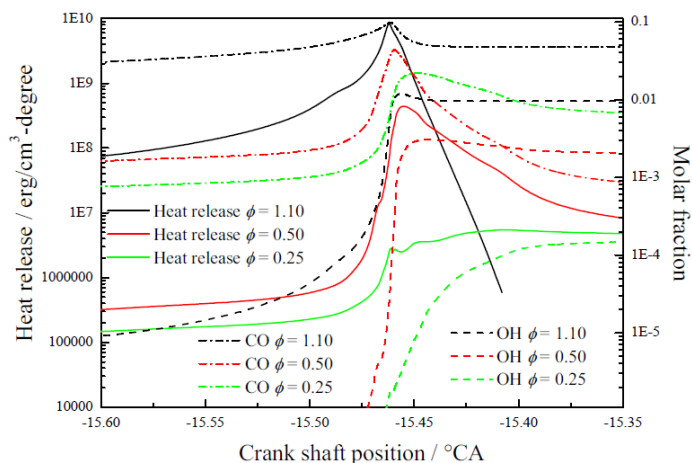


Figure 5. Heat release and species molar fraction as function of the crank shaft position – results for surrogate #1

4.2 Fuel surrogate #2 (toluene/i-octane/n-heptane/di-iso-butylene 45%/25%/20%/10% vol.)

For fuel surrogate #2 it was observed a numerical difference of the crankshaft position for maximum heat release in function of the stoichiometry, as seen on Figure 6. As in the case for fuel surrogate #1, on Figure 6 also can be observed that for rich conditions the maximum temperature value is higher when compared to lean mixtures, indicating that the detailed kinetics model is thermodynamically consistent.

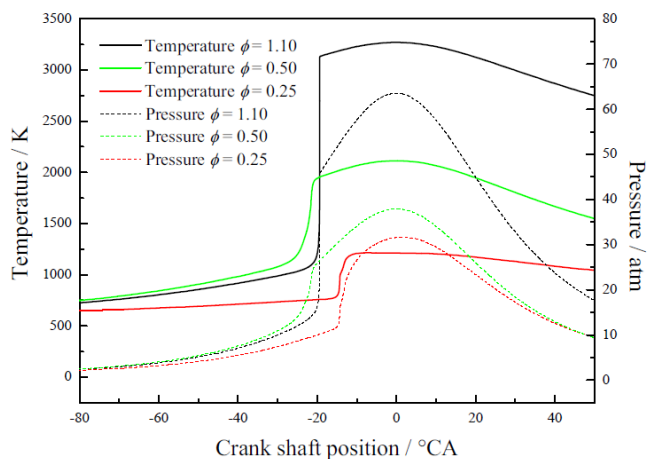


Figure 6 Temperature and pressure as function of the crankshaft position – results for gasoline surrogate #2

Figure 6 shows that there is a clear difference on times of ignition for the three stoichiometric conditions numerically tested.

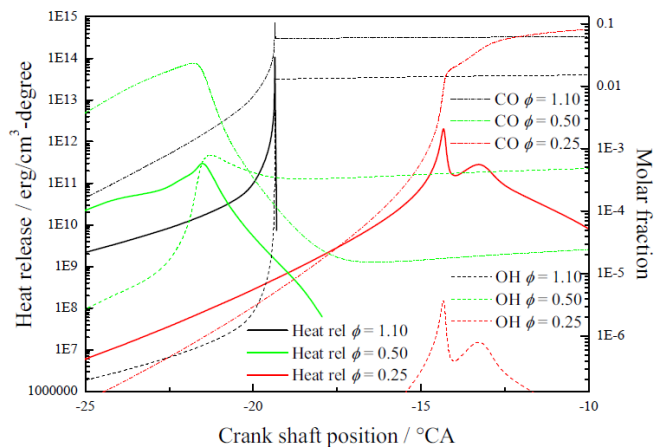


Figure 7. Heat release and species molar fraction as function of the crank shaft position – results for surrogate #1

The first one on exhibit autoignition is for stoichiometry of 0.5, followed by the rich mixture ($\Phi = 1.1$) and after the leanest mixture ($\Phi = 0.25$).

In terms of heat release and chemical species formation/depletion, the results observed on Figure 6 are consistent with the observed on Figure 7.

5. CONCLUSIONS

Although both the fuel surrogates formulations have similar RON/MON numbers (95.1/86.7 and 94.6/85), numerically were observed clear differences on the compression-ignition behavior. The fuel surrogate FS#2 has a big content of toluene (aromatic hydrocarbon) and this aspect involves a chemical behavior absolutely different when compared to the fuel surrogate FS#1. The other aspect is that FS#1 has an oxygenate hydrocarbon (alcohol, OH group) that will also make more distant the kinetics behavior.

In terms of initial temperature, it was necessary to increase the value for FS#2, and also increase the compression ratio (8.9 for FS#1 and 10 for FS#2) because that for values lower than those, the CHEMKIN return no-combustion. For higher values of compression ratio (12 and 13.5) the detailed kinetics model in combination with the CHEMKIN solver does not return a successful simulation, the CHEMKIN stop by non-convergence.

More detailed kinetics studies like sensitivity and reaction path analyses have to be performed in order to understand the difference of behaviors in terms of stoichiometry and ignition times.

6. ACKNOWLEDGEMENTS

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7. REFERENCES

- Andrae J.C.G., Björnbohm P., Cracknell R.F. and Kalghatgi G.T., 2007. "Autoignition of toluene reference fuels at high pressures modeled with detailed chemical kinetics". *Combustion and Flame*, Vol. 149, pp. 2–24.
- Cancino L.R., 2009. Development and Application of Detailed Chemical Kinetics Mechanisms for Ethanol and Ethanol Containing Hydrocarbon Fuels, Doctoral thesis, Federal University of Santa Catarina, Florianópolis, SC, Brazil.
- Cancino L.R., Fikri M., Oliveira A.M.M. and Schulz C., 2009. "Thermal Oxidation of Ethanol: experimental and Numerical Analysis of Ignition Chemistry of Ethanol-Air Mixtures in Shock-Heated Gases". 27th International Symposium on Shock Waves. St. Petersburg, Russia. Paper no. 30074.
- Curran H.J., Pitz W.J., Westbrook C.K., Callahan C.V. and Dryer F.L., 1998. "Oxidation of automotive primary reference fuels at elevated pressures". *Proceedings of the Combustion Institute*, Vol. 27, pp. 379–387.
- Hamilton, L., Rostedt, M., Caton, P., and Cowart, J., "Pre-Ignition Characteristics of Ethanol and E85 in a Spark Ignition Engine," *SAE Int. J. Fuels Lubr.* 1(1):145-154, 2009, doi:10.4271/2008-01-0321.
- Heywood, J.B. *Internal Combustion Engines Fundamentals*. New York: McGraw-Hill, 1988.
- Konnov A.A., 2000. "Development and validation of a detailed reaction mechanism for the combustion of small hydrocarbons". 28th Symposium (Int.) on Combustion, Edinburgh. WIPP Abstract pp. 317. Available as supplementary material. In: Konnov A.A. (Ed.), 2009. "Implementation of the NCN pathway of prompt-NO formation in the detailed reaction mechanism". *Combustion and Flame*, Vol. 156, pp. 2093–2105.
- Marinov N.M., 1999. "A detailed chemical kinetic model for high temperature ethanol oxidation". *International Journal of Chemical Kinetics*, Vol. 31, pp. 183–220.
- Maurice L.Q., 1996. Detailed Chemical Kinetic Models for Aviation Fuels. Ph.D. thesis, Imperial College, London, England.
- Mendiratta, R. and Pundir, B., "Preignition with High Olefin Fuels in a 2-Stroke SI Engine," *SAE Technical Paper* 932395, 1993, doi:10.4271/932395.
- Menrad, H., Haselhorst, M., and Erwig, W., "Pre-Ignition and Knock Behavior of Alcohol Fuels," *SAE Technical Paper* 821210, 1982, doi:10.4271/821210.
- Metcalfe W.K., Pitz W.J., Curran H.J., Simmie J.M. and Westbrook C.K., 2007. "The development of a detailed chemical kinetic mechanism for diisobutylene and comparison to shock tube ignition times". *Proceedings of the Combustion Institute*, Vol. 31, pp. 377–384.
- Obert, E.F. *Internal Combustion Engines*, 3rd edition, International Text Book Company, USA, 1955.
- Suga, T., Kitajima, S., and Fujii, I., "Pre-Ignition Phenomena of Methanol Fuel (M85) by the Post-Ignition Technique," *SAE Technical Paper* 892061, 1989, doi:10.4271/892061.

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