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An experimental and kinetic modeling study of auto-ignition and flame propagation of ethyl lactate/air mixtures, a potential octane booster

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Abstract

Spark ignition engines are one of the main technologies in the transport sector. The improvement and optimization of the fuels used to empower these engines are of vital importance, both for economic and environmental reasons. In particular, one of the main issues of spark ignition engines is the knock phenomenon; new formulations of fuels are being studied in order to overcome this problem. In this study, a possible innovative anti-knock, octane booster additive is considered: ethyl lactate. This molecule is almost unknown in combustion literature, as it has been used only as green solvent and food additive. The first experimental results under combustion conditions are presented, together with a kinetic mechanism. Two set-ups have been employed: a rapid compression machine, to measure ignition delay times, and an innovative spherical bomb, OPTIPRIME, to obtain laminar flame speeds. The results are encouraging for the expected application and the mechanism shows good performance. Ignition delay times at all conditions are well predicted by the mechanism and, when compared to ethanol, they are longer, implying a greater anti-knock capability. A rate of production analysis has been performed, where the unimolecular reaction leading to ethylene and lactic acid has been proved to be quite important at high temperatures and lean conditions. For laminar flame speeds, the agreement between model and experiments is good, with some discrepancies at lean conditions and high pressures. Compared to ethanol, at rich and stoichiometric conditions ethyl lactate flame speeds are slightly slower except at lean conditions, indicating that under some conditions this molecule could provide better performances than ethanol as an octane booster additive.

Keywords: ethyl lactate; octane booster; ignition delays; flame speed; kinetic modeling

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1. Introduction

Research for improved fuels in spark ignition engines is ongoing; anti-knock agents and high-octane fuels are of vital importance for these engines. Furthermore, the fact that the pollutant emission norms become more and more stringent, orients researchers towards new additives. Currently the most common additives are ethanol and methyl tert-butyl ether (MTBE), even if the latter has encountered problems related to ground water contamination. Other new options, such as 2-phenylethanol as proposed by Shankar et al [1], are being studied, with a special regard to sustainability and emission control. A list of potential octane boosters derived from biomass and an analysis of the physical characteristics expected from these compounds can also be found in [2].

Oxygenated additives proved of being capable of improving fuel volatility, enhancing the combustion efficiency and reducing CO and hydrocarbon emissions [3]. In this context, a new family, hydroxy esters, has caught interest. In particular, ethyl lactate may have the right characteristics to substitute ethanol as an octane enhancer and anti-knock additive in spark ignition engines. Also, when compared to the requirements listed in [2], it seems to have acceptable characteristics (like boiling and melting points, non-toxicity, solubility, etc) even if it was not included in that list.

Ethyl lactate ($C_5H_{10}O_3$) is an oxygenated compound, which is used as solvent and food additive [4, 5]. Its molecular structure is illustrated in Fig. 1.

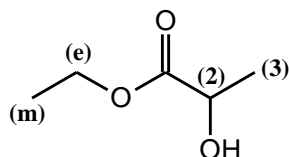


Figure 1. Ethyl lactate molecular structure (letters and numbers to identify the possible radical sites, the radicals are named accordingly in the mechanism)

Different production processes have been proposed with continuous improvements, due to the promising characteristics of this molecule. The most common production process is esterification of lactic acid with ethanol, catalyzed by an acid, as presented by Pereira et al. in [5], while new pathways have been explored by Li [6] and Koutinas [7]. All these processes require

Table 1. Comparison of ethyl lactate characteristics with other octane boosters for gasoline [1, 2, 8, 9]

	Ethanol ⁽¹⁾	Ethyl lactate ^(7,8)	Ethyl butanoate ^(2,9)	MTBE ^(7,8)
Molecular formula	C_2H_6O	$C_5H_{10}O_3$	$C_6H_{12}O_2$	$C_5H_{12}O$
Density ($kg L^{-1}$)	0.784	1.031	0.874	0.7405
Molar mass ($kg mol^{-1}$)	0.046	0.118	0.116	0.088
Heat of vaporization ($kJ kg^{-1}$)	918.20	416.95	339.66	339.77
Flash point ($^{\circ}C$)	14	46	19	-33
Boiling point ($^{\circ}C$)	78.35	154	121	55.1

products from renewable resources, which is one of the positive aspects of ethyl lactate. Table 1 shows a comparison of ethyl lactate characteristics with two other known octane boosters, ethanol, and MTBE, and ethyl butanoate, one of the potential molecules proposed in [2].

To the best of the authors' knowledge, in the literature, there are no studies on the combustion characteristics of ethyl lactate. In this study, experiments were done in a rapid compression machine (RCM), where ignition delays of ethyl lactate/air mixtures are measured, and in OPTIPRIME set-up [10] for the measurement of laminar flame speeds in air. A kinetic mechanism was developed as well, in order to represent the results and to better understand the characteristics of this potential gasoline additive under engine-relevant conditions.

2. Experimental details

2.1 Ignition delay times

Ignition delay times (IDT) were measured using the RCM at PRISME. Experimental conditions are listed in Table 2. For all the conditions, the tests have been performed in "air" (21% O_2 /79% inert gases), with the inert being N_2 , Ar or a mixture of the two.

Table 2. Experimental conditions in the RCM.

ϕ	P (bar)	T (K)
0.5	20	822–919
1	20	824–920
	30	827–928
1.5	20	788–885

2.1.1 Rapid compression machine

A thorough description of the RCM set-up at PRISME can be found elsewhere [11], here just a brief summary is provided. The machine is equipped with one piston, which is pneumatically driven and hydraulically controlled. The stroke length of the configuration used for this application is 300 mm and the volumetric compression ratio used is between 8 and 9. The piston has been manufactured with a creviced head, in order to prevent vortex roll-up and therefore ensure the homogeneity of the core gas [12–14]. This allows the use of the adiabatic core hypothesis to compute the condition at the end of compression (TDC, top dead center in the cylinder).

A piezoresistive transducer (AVL QC34C), the characteristics of which can be found in [15], is used to measure the pressure inside the cylinder. The intake temperature measurement is performed through a type K thermocouple (accuracy $\pm 1\text{K}$). The mixture of gases is prepared in a separated tank, continuously stirred and heated in order to prevent condensation and insure homogeneity. At all stages of the experiments the saturation temperature was computed from Antoine's equation and a safe margin in the employed temperature was always assured.

2.1.2 Experimental methodology and evaluation

The typical pressure profile from an RCM experiment is illustrated in Figure 2.

Pressure profiles from reactive mixtures are used to determine the ignition delay time, defined as the time between the end of the compression (TDC) and the maximum of the time derivative of the pressure (dP/dt).

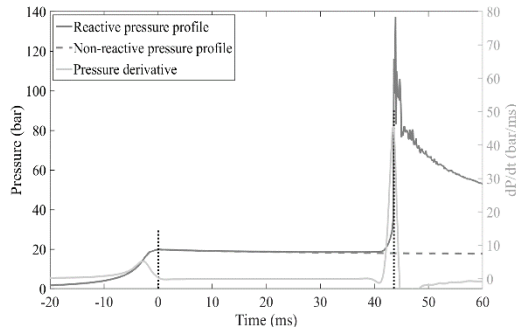


Figure 2. Typical pressure traces from RCM experiments ($\phi = 1.5$, $T_c = 837\text{ K}$, $P_{TDC} = 19.82\text{ bar}$, diluent 100% Ar)

The pressure at the end of the compression is measured, while the temperature can be computed with the hypothesis of adiabatic core, i.e. using the isentropic formula:

$$\ln\left(\frac{P_c}{P_0}\right) = \int_{T_0}^{T_c} \frac{\gamma}{\gamma-1} \frac{dT}{T} \quad (1)$$

where the subscripts 0 and C indicate respectively initial and end-of-compression conditions, T is the temperature, P the pressure and γ the temperature dependent heat capacity ratio of the mixture.

Traces from non-reactive mixtures are used to account for heat losses for the simulations through the computation of volume time histories, which are specific to our facility and the used mixture. Oxygen is replaced by nitrogen, in order to maintain the thermodynamic characteristics of the mixture, without auto-ignition.

2.2 Laminar flame speeds

Flame speeds were measured in the OPTIPRIME set-up in ICARE. The experimental conditions of these experiments are reported in Table 3. In these experiments, mixtures in air (79% N_2 and 21% O_2) were tested.

Table 3. Experimental conditions in OPTIPRIME.

Dilution	ϕ	P_0 (bar)	T_0 ($^\circ\text{C}$)
Air (21% O_2 /79% N_2)	0.7	1, 2, 3	135
	1	1, 2	135
	1.2	1	135

2.2.1 OPTIPRIME

OPTIPRIME is a spherical bomb set-up, designed to measure flame speeds under different conditions. A complete description is found elsewhere [10], here only a brief description is given. OPTIPRIME is a perfectly spherical isochoric combustion chamber with full optical access, which allows the simultaneous recording of the pressure and the flame radius from the ignition point until the wall. It is made by two stainless steel half shells, with a 360° fused silica ring; the quartz thickness is 11 mm, which ensures resistance to pressure greater than 100 bar. The total volume of the chamber is 0.943 L, a quite small volume which ensures an easier homogeneous pre-mixture and reduces the effects of radiation and hydrodynamic instabilities. The sphere is equipped with two pressure sensors with high sensitivity and frequency; a type K thermocouple is introduced in the chamber to check the initial temperature. The whole sphere is placed inside a furnace, in order to avoid inhomogeneity in the temperature; the operative range of the furnace is between 10 to 200°C . The mixture to be tested is prepared in a separate tank; in the case of liquid fuel, as ethyl lactate, this is injected directly in the sphere using a high-precision syringe, to avoid condensation in the buffer tank, since that is not heated. Finally, the mixture is ignited thanks to an electric discharge between two ultra-fine electrodes (0.35 mm in diameter) and the images are recorded. The camera used was PHANTOM V1611 operating between 8000 to 15000 fps. In order to limit optical deformations, a calibration of the system is performed before the testing.

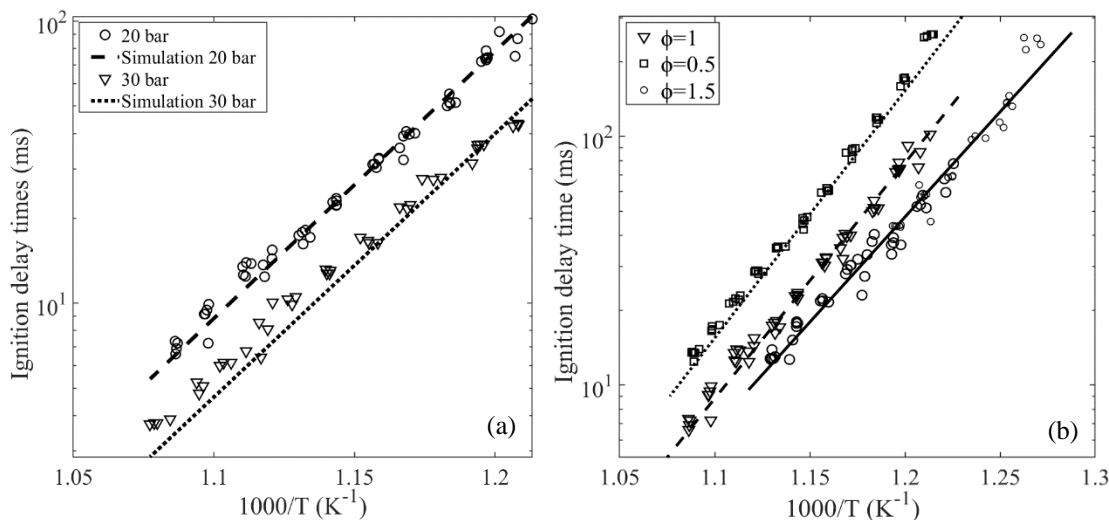


Figure 3. Ethyl lactate ignition delay times, experimental results (symbols) vs simulations (lines); a) $\phi = 1$, $P = 20$ and 30 bar, b) $P = 20$ bar, and $\phi = 0.5$, 1 and 1.5

3. Modeling and simulations

A new mechanism for ethyl lactate combustion has been developed; no other kinetic mechanisms could be found in the literature for comparison.

As a starting point, a sub-mechanism for ethanol available in ICARE database has been used; then, specific reactions for ethyl lactate, its radicals and its main products (as for example lactic acid, glycolic acid, ethyl pyruvate) have been added. When available, Arrhenius parameters for the rate constants have been taken for the specific molecule and reaction; in the other cases, analogies were made.

- H-abstraction reactions by H atoms and CH_3 radicals have been taken from Wurmel et al [4].
- H-abstraction rate constants by HO_2 radicals from carbon (2) were estimated by similarity to isopropanol as in [16] and were multiplied by 4 to take into account the carbonyl group, while the same abstraction by OH has been taken from the calculation of Mendes et al [17] for iso-butanol.
- Rate constants of H-abstraction reactions from carbon (e) by HO_2 radicals were estimated by similarity from the ones proposed by Zhou et al [18] for n-butanol, multiplied by 2, while the rate parameters for H-abstraction from the same site by OH radicals was taken as similar to diethyl ether [19].
- The rate constant for the unimolecular reaction $\text{C}_3\text{H}_{10}\text{O}_3 \rightarrow \text{C}_2\text{H}_4 + \text{C}_3\text{H}_6\text{O}_3$ was taken as equal to that for propyl acetate [20]. The same rate constant was used also for the unimolecular reactions of ethyl lactate products (ethyl pyruvate, ethyl glycolate).
- β -scission reactions of ethyl lactate radicals were estimated by analogy with similar radicals: 1-pentanol radicals [21], ethyl acetate radicals [22], and butyl formate radicals [23].

The complete mechanism can be found in the supplementary material.

All simulations, both for ignition delay times and laminar flame speeds, were performed using ChemkinPRO [24]. The homogeneous reactor model was used for the rapid compression machine simulations, with the volume-time profiles computed from tests for non-reactive mixtures. PREMIX module was used for laminar flame speed simulations, with the implementation of a parametric study over the pressure and temperature range, assuming an isentropic evolution of the conditions.

4. Results

4.1 Ignition delay times

At all conditions, ignition delay times decrease with increasing temperature, as expected. No negative temperature coefficient zones are encountered for any of the studied conditions, showing that ethyl lactate is not presenting a significant low temperature reactivity. Increasing the pressure and the equivalence ratio result in a decrease in the ignition delay times over the whole temperature range.

Figure 3a illustrates the experimental results and simulations results for $\phi = 1$, at 20 and 30 bar, while in Figure 3b the results for three different equivalence ratios at the same experimental pressure are shown. At all conditions, the model shows very good performance, with a maximum deviation of 28% at $\phi = 1$ and a compressed gas pressure of 30 bar.

4.1.1 Rate of production analysis

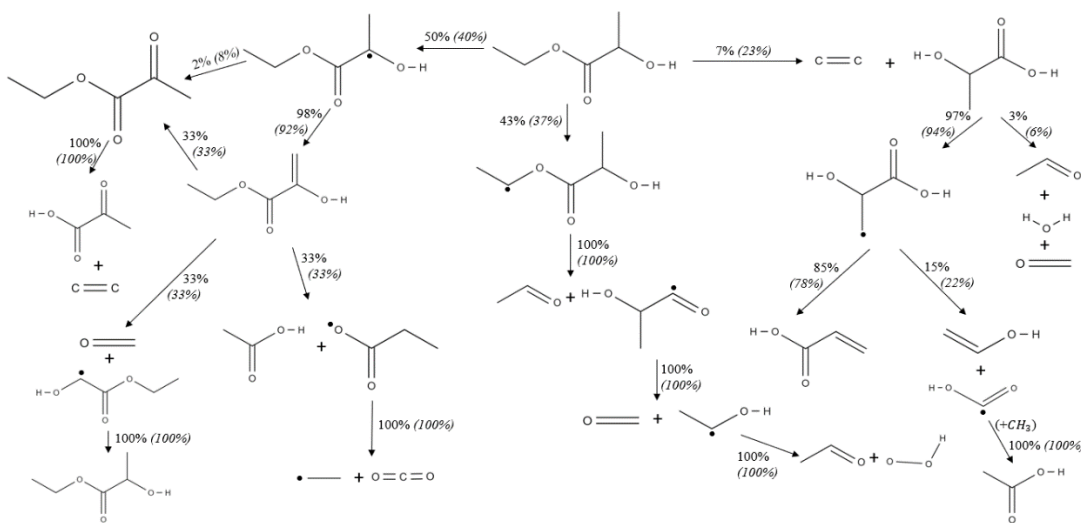


Figure 4. Reaction pathways in ethyl lactate oxidation. Conditions: $\phi = 1$, $P = 20$ bar, at 830 K and 915 K (italics in parenthesis)

A reaction path analysis was done at the time for which the fuel consumption reaches 20% and is presented in Figure 4. It can be seen that the reaction paths are the same at the lower and higher temperatures, only the relative importance of the reactions is slightly different. In particular, the fuel is consumed mainly by H-abstraction, on the (e) and (2) sites by HO_2 and OH radicals; while fuel decomposition via unimolecular reaction producing ethylene and lactic acid ($\text{C}_5\text{H}_{10}\text{O}_3 \rightarrow \text{C}_2\text{H}_4 + \text{C}_3\text{H}_6\text{O}_3$) represents 7% and 23% at 830 and 915 K, respectively.

Although not presented in Fig. 4, at $\phi = 0.5$, and around 920 K, this percentage increases up to 31%, while at 880 K and $\phi = 1.5$, the same reaction accounts only for 12% of ethyl lactate consumption. From these numbers, it is possible to infer that the unimolecular reaction $\text{C}_5\text{H}_{10}\text{O}_3 \rightarrow \text{C}_2\text{H}_4 + \text{C}_3\text{H}_6\text{O}_3$ has a non-

negligible role in ethyl lactate consumption at high temperatures and lean conditions. Among the main reaction products, it is interesting to note the production of ethyl pyruvate, which is totally consumed by the unimolecular reaction leading to ethylene and pyruvic acid. On the other hand, lactic acid, mainly undergoes H-abstraction, followed by decomposition into propenoic acid (85%) and ethenol plus the hydrocarboxyl radical (15%).

4.1.2 Comparison with ethanol

In order to assess the possibility of using ethyl lactate as an anti-knock additive in spark ignition engine, as an alternative to ethanol, a comparison of the ignition delay times between the two fuels is performed. Using the same RCM, ignition delay times of ethanol are measured, in comparable conditions: $\phi = 1$, TDC pressure = 20 bar and within a temperature range of 815–890 K.

As can be seen in Figure 5, ethyl lactate has slightly longer ignition delay times, which is a suitable characteristic for an additive of this kind. This would mean that a lower quantity of this additive would be needed compared to ethanol, in order to obtain the same effect on the final mixture. Moreover, considering that ethyl lactate has a heat of vaporization which is less than a half of that of ethanol, but very close to the that of common gasoline, this molecule is a really promising additive for spark ignition engines, since it is very likely to be exploitable without major modifications to the current engines.

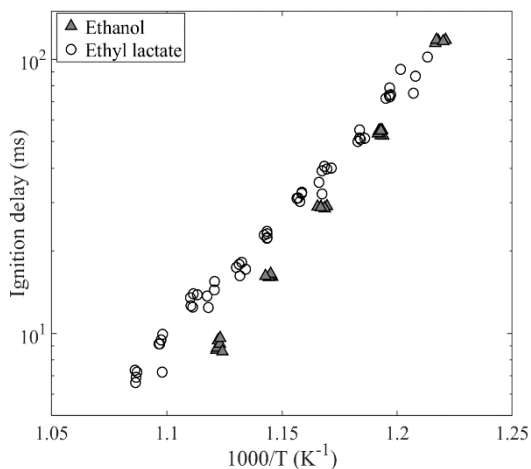


Figure 5. Ethanol vs ethyl lactate ignition delay times at $\phi = 1$, $P_c = 20$ bar (in air)

4.2 Laminar flame speeds

The experimental results obtained in OPTIPRIME setup and the performed simulations are plotted in

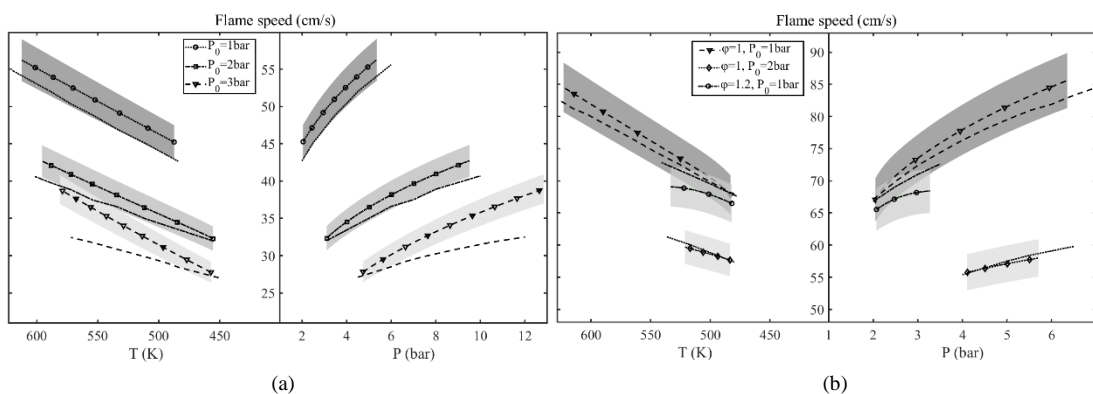


Figure 6. Laminar flame speeds: a) $\phi = 0.7$, initial pressures of 1, 2, 3 bar, b) $\phi = 1$ at 1 and 2 bar, and $\phi = 1.2$ at 1 bar, (lines with symbols indicate experimental results, simple lines (solid or dashed) simulation results)

Figure 6. Thickened traces correspond to experimental results with their associated uncertainty ($\pm 5\%$) [25]. It is important to consider that these results were obtained in an innovative set-up, which allows to measure flame speeds under isochoric conditions, with pressure and temperature that increase together isentropically during the experimental run. Therefore, as can be seen from the figure, flame speeds can increase with increasing pressure, because at the same time there is an increase in the temperature. Considering the experimental results in Figure 6a, for the $\phi = 0.7$ mixture and for an initial temperature of 408 K, a higher initial pressure leads to slower flame speeds over the whole isentropic development of the flame. For all conditions, when the temperature is increased along with the pressure, the flame speed increases, even if the slope appears to be different for the different conditions. From Figure 6b, it can be observed that the flame speeds at $\phi = 1.2$ are slower than the ones obtained under stoichiometric conditions. The mechanism can reproduce these results well, with flame speeds very similar for these two equivalence ratios at low temperatures, but more and more different as

temperature increases. In the case of $\phi = 1.2$, there are less experimental data, due to flame instabilities at higher pressures. For the lean conditions, the model is performing well at lower initial pressure, while there is a higher disagreement with the experiments starting at an initial pressure of 3 bar, with a maximum error around 15% at high temperature. In particular, it is interesting to note that the slope of the flame speed evolution over the pressure range is well predicted by the model in the case of initial pressure of 1 bar, while deviations are observed for the higher initial pressures, leading to a fair prediction of flame speed values in the first part, but less accurate at higher temperatures.

4.2.1 Sensitivity analysis

In order to have a deeper insight in the reactions having the highest impact in ethyl lactate/air laminar flame speeds, a sensitivity analysis on the flow rate has been performed (Figure 7).

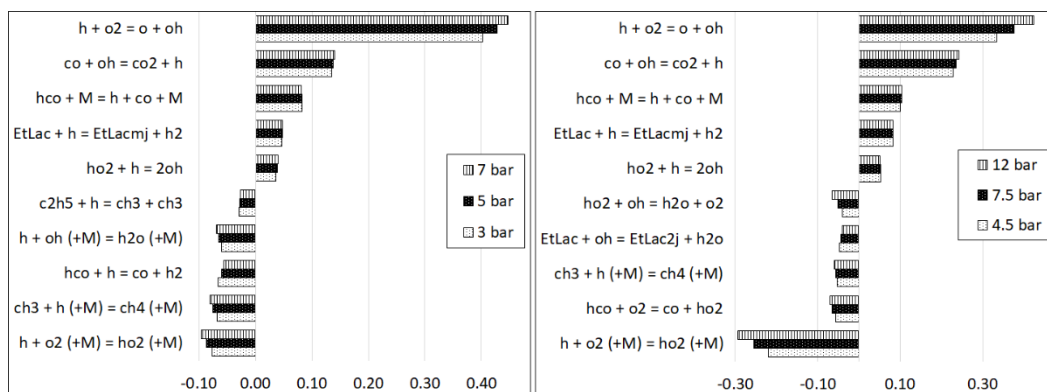


Figure 7. Laminar flame speed sensitivity analysis: left panel: $\phi = 1$, $P_0 = 1$ bar, right panel: $\phi = 0.7$, $P_0 = 3$ bar.

A condition for which the model is performing well is considered ($\phi = 1$, initial pressure 1 bar), as well as the most problematic ($\phi = 0.7$, initial pressure 3 bar), in order to compare the most important reaction in flame speeds determination. In both cases, the competition between the reaction $\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$ and $\text{H} + \text{O}_2 (+\text{M}) \rightleftharpoons \text{HO}_2 (+\text{M})$ has a strong effect, as expected. The rate constants for these two reactions have been adopted as the ones proposed by Stagni et al [26] which seem to properly describe this competition [27]. Another reaction showing an important effect for both conditions is the reaction $\text{CO} + \text{OH} \rightleftharpoons \text{CO}_2 + \text{H}$, for which the rate parameters are adopted from Davis [28]. Although the sensitivity analysis for rich condition is not reported here, this reaction is especially sensitive at $\phi = 1.2$. An important reaction for stoichiometric and rich conditions appears to be $\text{HCO} + \text{H} \rightleftharpoons \text{CO} + \text{H}_2$. In this study, the rate coefficients of this reaction were taken from the NUIG 1.1. mechanism [29]. This reaction is very sensitive especially because it has an inhibiting effect on rich and stoichiometric conditions, without greatly impacting the lean conditions, where flame speeds are already under-predicted.

Lastly, it is interesting to consider the reaction where ethyl lactate directly takes part. In all conditions of this experiment, the H-abstraction reaction by H atoms on site (m) has a promoting effect on the flame speed. This impact is more important at lean conditions and higher pressure ($S = 8.18 \times 10^{-2}$ for $\phi = 0.7$, $P_0 = 3$ bar), while it is much less sensitive in the rich condition (for $\phi = 1.2$, the computed sensitivity coefficient is 3.26×10^{-2}). On the other hand, the H-abstraction reaction from the (2)-site by OH radicals has an inhibiting effect ($S = -4 \times 10^{-2}$, and slightly pressure dependent) for the lean mixture, while it does not appear among the most important reactions in rich and stoichiometric conditions. In all the conditions studied, the unimolecular reaction identified as an important fuel consuming reaction in ignition delay measurements does not seem to have a strong influence on the flame speed.

4.2.2 Comparison with ethanol

In addition, a comparison with ethanol can be useful to have a reference point for the characteristics of this new possible additive for spark ignition engines. Obtaining comparable results for flame speeds is not as obvious as it is for ignition delay time. In fact, even if several experimental results are available for ethanol, none of these are showing an evolution over the pressure as the ones obtained in the OPTIPRIME set-up. Therefore, in order to have a proper comparison, the correlation for ethanol laminar flame speeds reported by Liao et al [30] is used to compute the ethanol flame speed at 408 K. For ethyl lactate, data obtained by an isobaric treatment accounting for the stretch effects at 1 bar and $T_0 = 408$ K are used.

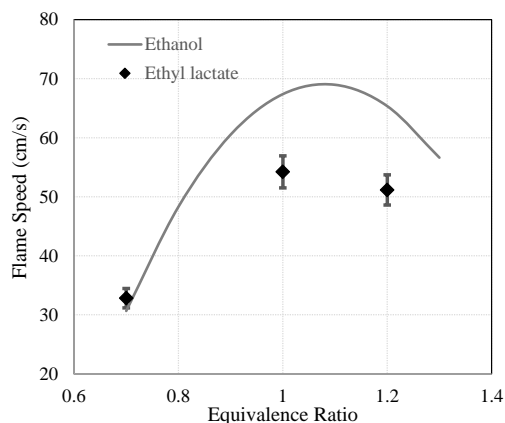


Figure 8. Ethanol vs ethyl lactate flame speeds at $P = 1$ bar, $T_0 = 408$ K (ethyl lactate flame speeds come directly from our measurements, while ethanol flame speeds are computed thanks to the correlation proposed by Liao et al [30]).

The result of this comparison can be seen in Figure 8. Ethyl lactate has slower flame speeds at rich and stoichiometric conditions. At lean conditions, the laminar flame speeds of both fuels are comparable (ethyl lactate slightly faster by about 5%). Therefore, even if ethyl lactate is not always providing higher laminar flame speeds, in lean conditions it can possibly be a convenient alternative for some applications.

5. Conclusions

The aim of this work was to provide some first experimental data on the combustion behavior of ethyl lactate, a possible anti-knock additive for spark ignition engine. For this reason, experiments in a rapid compression machine and in OPTIPRIME, an isochoric spherical bomb, have been performed. The second goal was to obtain a first kinetic mechanism, for which no previous work was available in the literature.

The results obtained in the present study are quite promising. The model showed a good performance both for ignition delay times and laminar flame speeds simulations. In addition, the experimental results themselves are interesting for the foreseen application. Ethyl lactate has higher resistance to auto-ignition than ethanol under engine-relevant conditions and hence can be used in less quantities than ethanol if considered as an octane booster, and in the meantime has comparable laminar flame speeds under lean conditions. The global combustion characteristics of ethyl lactate seem to be very interesting for a future use as an anti-knock and octane booster additive.

The major limitation on the performance of the present model seems to be found at lean conditions for

laminar flame speeds. As a perspective, in order to constrain the C₀-C₂ chemistry in the model, smaller molecules will be studied. Experiments will be performed for laminar flame speeds in OPTIPRIME and further improvements can be brought in order to improve the performance of the whole model.

Acknowledgements

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Supplementary material

The kinetic mechanism, thermochemistry file as well as the experimental data are provided as supplementary material.

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