73rd Conference of the Italian Thermal Machines Engineering Association (ATI 2018), 12-14 September 2018, Pisa, Italy

Development of a chemical-kinetic database for the laminar flame speed under GDI and water injection engine conditions

Giulio Cazzoli[a,*], Stefania Falfari[a], Gian Marco Bianchi[a], Claudio Forte[b]

[a]University of Bologna, V.le del Risorgimento 3, Bologna 40131, Italy
[b]NAIS Engineering, Address, City and Postcode, Country

Abstract

The use of direct injection, supercharging, stoichiometric operation and reduction of the engine displacement, necessary to limit the specific consumption without reducing the power, makes the current spark ignition engines sensible to both the detonation and the increase of the inlet turbine temperature. The current research has therefore focused on the study of strategies aimed at reducing the risk of detonation using traditional and innovative solutions such as water injection. The application and optimization of these strategies can not ignore the knowledge of physical quantities characterizing the combustion such as the laminar flame speed. The laminar burning speed is an intrinsic property of the fuel and it is function of the mixture composition (mixture fraction and dilution) and of the thermodynamic conditions. The experimental measurements of the laminar flame speed available in the literature, besides not being representative of the pressure and temperature conditions characteristic of GDI engines, rarely report the effects of dilution by EGR or water vapor. To overcome the limitations of the experimental campaign it is possible to predict the value of the laminar flame speed resorting to numerical combustion models based on chemical kinetics. The increased performance of computing systems makes affordable the use of chemical schemes with a high number of species and reactions without facing an excessive temporal cost. In this work it is presented a methodology for the construction of a laminar flame speed database based on a non-reduced kinetic scheme and an open source solver (Cantera) for a commercial gasoline surrogate under the typical conditions of GDI engines with the addition of the effects of dilution with water and EGR.

Keywords: Chemical kinetics; Laminar flame speed; Diluent effect; GDI engine

1. Introduction

The laminar flame speed (LFS) is a fundamental property that characterize an oxydizer-fuel mixture in terms of reactivity, diffusivity and exothermicity. This property depends on the fuel composition and on the mixture quality,

*Corresponding author. Tel.: +39-0512093316
E-mail address: giulio.cazzoli@unibo.it

expressed by equivalence ratio and dilution, and its thermodynamic state. The LFS has a fundamental role in modeling combustion process [1].

It is well established that adding a diluent to a reactive mixture leads to a significant change in the flame properties, not only due the pure dilution effect, but also for thermal and chemical effects. In Diesel engines the use of the charge diluition with residual gases is an established method for pollution control (for example see Ladommatos et al. [2] or Bianchi et al. [3]). The use of water as combustion control technique has a long history [4], for pollution control (for example Kohketsu et al. [5]), increase in performance or component protection. Traditionally reserved for large engines or combustors, recently it has been considered for use in small ignition engines as the actual GDI (gasoline direct injection) SI (spark ignition) engines, moving toward downsizing, are more exposed to knock and preignition risks. It must also considered that engine stoichiometrich operations at full load is becoming mandatory in RDE vehicle test cycle. One of the promising strategy to increase efficiency, reduce the detonation risk at high load and to achieve turbine protection is to use water in addition to the conventional dilution with exhaust gas (exhaust gas recirculation, shortly EGR) [6, 7]. This results in the need to accurate estimate LFS of water diluted air/fuel mixtures.

The definition of LFS requires that an experimental apparatus used to measure it operates with gaseous flow under laminar regime (see Rallis et al. [8] for an in-depth survey). This results in severe limitations on the type of fuel and on both the mixture thermophysical conditions and quality. For fuel in liquid form at ambient condition, like the heavy hydrocarbons, the necessary preheating atomization and vaporization [9] limit the minimum obtainable temperature. High temperature and pressure are limited by the intrinsic structure of the apparatus (most of the flame tests are in open atmosphere), and by the rapid insurgence of the flame instability, which worsen at rich conditions [10].

In order to overcome this limitation and define a value for the LFS for the condition characterizing the combustion process in IC engine, a correlation, usually a power law (for early works see Gilbert [11] or Metghalchi [12]), is defined using the available experimental data: then it is extrapolated well beyond the defined experimental space.

Alternatively, LFS can be obtained numerically using the principles of chemical kinetics. The quality of the result depends on the complexity of the used kinetic scheme, complexity that results in long calculation times. The rapid increase in readily available computing power has made possible the use of complex patterns.

In a previous paper the authors defined and validated a chemical kinetics methodology that permits to extimate the LFS of a gasoline-like surrogate under engine-like thermophisical conditions ([13]). To provide the necessary support to the numerical analysis of the combined use of water and EGR as detonation prevention mechanism presented by Falfari et al. [14], the same methodology has been expanded in order to include the effect of dilution with EGR and water.

2. Numerical approach

The computational approach proposed in [13] uses the 1D adiabatic flame solver provided by Cantera [15] (version 2.3), an open-source library for problems involving chemically-reacting flows. The original code has been improved with the introduction of two diluents, both defined as mass fraction in relation to the total mass of air and diluents. The composition of the water-diluent is, obviously, pure water in gaseous form. The composition of the EGR-diluent is defined with the typical constituents CO_2, H_2O and N_2 obtained from the stoichiometric combustion of the chosen fuel at the prescribed equivalence ratio.

The correct implementation of the dilution with water has been validated using the experimental data for methane measured by Mazas et al. [16]. Mazas reports the experimental values of the LFS for methane at atmospheric pressure and temperature with equivalence ratio from 0.5 to 1.6. The effect of the water dilution, defined as molar fraction up to 0.2, are measured at stoichiometric equivalence ratio and with an unburned temperature of 473 K, in order to allow the addition of gaseous water and to stabilize the flame. A methane data-set has been chosen due the lack of LFS measurement of heavy hydrocarbon with water as diluent and for the almost standard GriMech [17] chemical kinetic mechanism. As expected, the GriMech mechanism, at ambient conditions, (figure 1a) calculates with sufficient accuracy the value of the LFS (S_L) as a function of the equivalence ratio (φ). In figure 1b one can see that the effect, according to the proposed approach, of the water dilution correctly matches the experimental data. As it can be seen in figure 1c, the combined effect of dilution with water and non stoichometric mixture is far from being linear and practically it is non-existent for rich and lean mixtures, in agreement with what reported by Mazas.
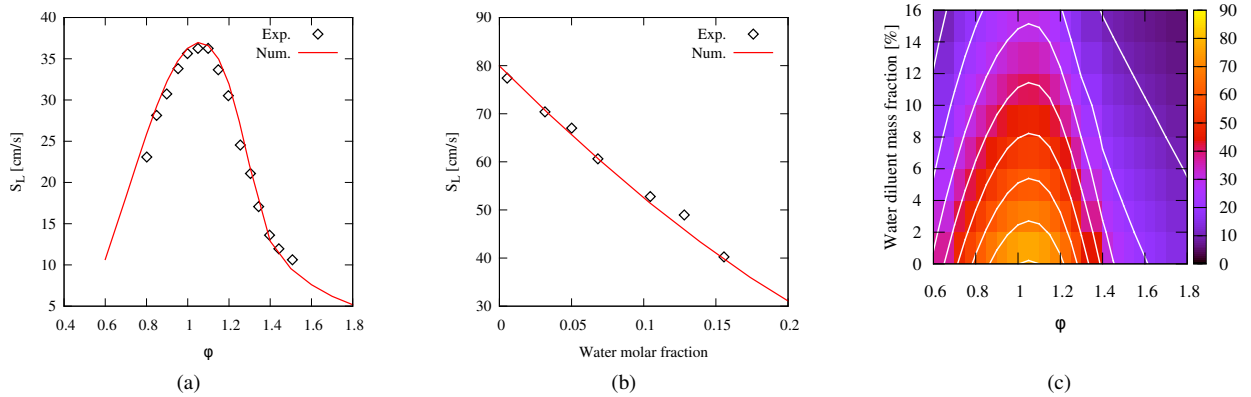
Figure 1: Methane's LFS at ambient pressure, temperature of the unburned 473 K. (a) Effect of the equivalence ratio for an undiluted mixture. (b) Effect of the water dilution at $\varphi = 1$. (c) Combined effect of φ and water diluent, numerically evaluated. Experimental data from Mazas et al. [16].

3. LFS for gasoline surrogate at different conditions

The quality of the numerical LFS predictions depends on the employed kinetic reaction scheme. The majority of chemical mechanisms available are composed of elementary sets of reactions, validated against extensive data. In the author's previous work [13], after an extensive validation, the semi-detailed mechanism proposed by the CRECK group [18], composed by 251 species and 8200 reactions has been chosen as reference mechanism for the simulation of laminar flame speed of a fuel (RON 98.1, composed by 13.7% (vol.) n-heptane, 42.9% iso-octane, 43.4% toluene, in the following named TAE) proposed by Dirrenberger [19] as surrogate of a commercial gasoline with RON 95.6.

3.1. Numerical spaces

The proposed methodology has been used to assess the effects on the laminar flame speed under the typical conditions encountered during the combustion process in a modern GDI engine: high pressure, high temperature, mixtures from very lean to very rich, dilution of the fresh charge. Three different space has been considered: a four-dimension space (Table 1), defined in order to highlight the effect the traditional dilution that use only EGR up to very high values. A five-dimension space (Table 2), defined in order to highlight the combined effect of EGR and water dilution, the maximum diluent mass fraction for both component has been chosen according the knock prevention strategy following Falfari et al. [14]. Lastly a three-dimension space has been defined to asses the effect of dilution at reference pressure and temperature (1 bar and 358 K respectively). It must be observed that the unburned temperature has been limited in order to avoid the non-physical results observed in [13].

3.1.1. LFS analytic correlation

The tabulated space can be directly used by local linear interpolations. Alternatively, a LFS correlation can be defined by the tabulated space in order to grant a faster access to the laminar flame speed's value with a low memory

Table 1: Engine-like thermopysical condition, High EGR space

	Range	Step size
φ	0.4-2.0	0.1
Pressure	90-290 bar	40 bar
Temperature	400-700 K	100 K
EGR	0-30%	5%

Table 2: Engine-like thermopysical condition, Water injection space

	Range	Step size
φ	0.4-2.0	0.1
Pressure	90-290 bar	40 bar
Temperature	400-700 K	100 K
EGR	0-6%	1%
Water	0-6%	1%

cost. The use of a correlation can lead to loss of accuracy or some unphysical effect due to chosen model and fitting procedure. Following the work of other authors (for example Metghalchi [12]) for a given value of LFS at undiluted reference conditions ($S_{L,0}(\varphi)$), the value of LFS can be computed for every condition, considering the diluition effect, with:

$$S_L(\varphi, T_u, p_u) = S_{L,0}(\varphi)\left(\frac{T_u}{T_0}\right)^{\alpha(\varphi)}\left(\frac{p_u}{p_0}\right)^{\beta(\varphi)} f(x_{dil}) \tag{1}$$

where T_0 and p_0 are temperature and pressure value at reference condition and $f(x_{dil})$ is a function, usually a linear one, of the diluent mass fraction (x_{dil}). The power coefficient α and β usually are constant or linearly dependent from the equivalence ratio.

In [13] a correlation in the form of equation (1) has been successfully fitted over a similar engine-like space (without dilution and for $\varphi \leq 1.8$). In the proposed correlation the LFS at the reference condition ($S_{L,0}$) was:

$$S_{L,0}(\varphi) = a\, e^{-(\varphi-\varphi_m)^2/b} + c\,\varphi + d\,\varphi^2 \tag{2}$$

and both the power coefficient α and β are in the form:

$$\alpha = a_0 + a_1\varphi + a_2\varphi^2 + a_3\varphi^3 \qquad\qquad \beta = b_0 + b_1\varphi + b_2\varphi^2 + b_3\varphi^3 \tag{3}$$

In this work the diluent effect will be introduced with a linear term as follows:

$$f(x_{EGR}, x_{wat}) = (1 - k_e\, x_{EGR})(1 - k_w\, x_{wat}) \tag{4}$$

where x_{EGR} and x_{wat} are the mass fraction of EGR and water, respectively. It should be noted that the introduction of dilution with the product of two linear terms indirectly provides a cross-effect between the concentrations of water and EGR.

All the required coefficients were obtained by fitting the correlation against the relevant data with a nonlinear least-squares (NLLS) Marquardt-Levenberg algorithm. Following Galmiche et al. [20], firstly the coefficients for $S_{L,0}$ will be estimated for the reference condition, assumed at the experimental data value ($T_0 = 358$ K and $p_0 = 1$ bar). Then α and β, assumed to be dependent on the equivalence ratio (according to equation (3)), were simultaneously fitted using the wide range of temperature and pressure values. Lastly the EGR (k_e) and water (k_w) coefficient are determined.

3.2. LFS at reference conditions

Following the result presented in [13], at reference condition, the φ-LFS correlation shows an almost Gaussian shape in the range from lean up to rich mixture, after that the LFS assumes an almost asymptotic trend (Undiluted curve in figure 2a) without crossing the zero-speed line. Lacking an experimental confirmation it is reasonable to suppose that the flame is not able to sustain itself at extreme rich conditions.

The effect of dilution with pure EGR and pure water are also depicted in figure 2a. It's interesting to note that the dilution effect depends on the quantity of the diluent and on its quality. As can be seen in figure figure 2a, the same mass fractions of pure EGR and pure water produce a different reduction of LFS. Both dilutions reduce the LFS with an almost linear dependency. The combined effect of the two diluent shows no cross effect (figure 2b).
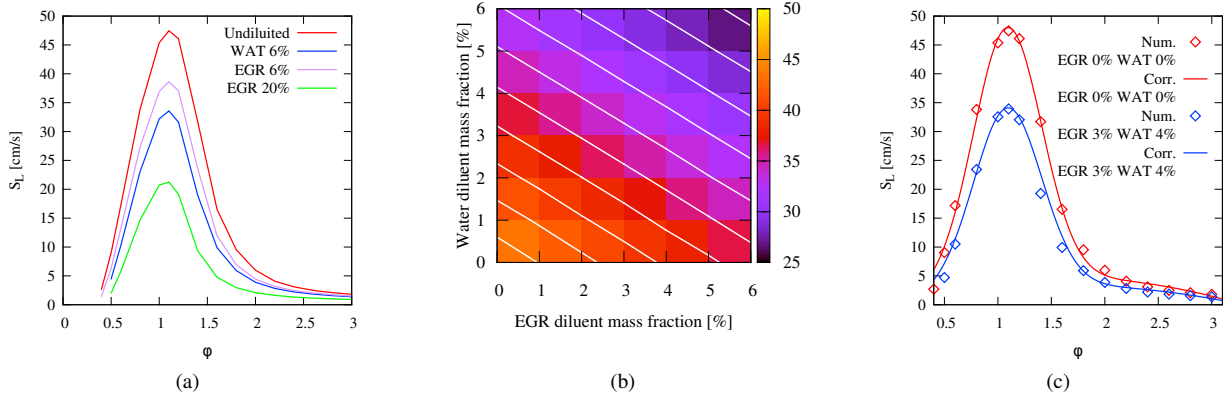
Figure 2: TAE's LFS at reference conditions. Effect of dilution: (a) Pure diluent, (b) Combined effect of EGR and water, (c) Correlation

3.2.1. Analytic correlation

The correlation between the LFS and the equivalence ratio, proposed in [13] for an undiluted case up to $\varphi = 1.8$, has been extended to the high equivalence ratio values. At reference condition, the undiluted LFS (equation (2)) with the effect of EGR (up to $x_{EGR} = 0.20$) and water (up to $x_{wat} = 0.06$) becomes:

$$S_{L,0}(\varphi) = \left(43.927\, e^{-(\varphi-1.0908)^2/0.20102} + 5.6289\,\varphi - 1.7110\,\varphi^2\right)(1 - 3.0893\,x_{egr})(1 - 5.6405\,x_{egr}) \qquad (5)$$

As can be see in figure 2c the correlation correctly reproduce the effect on LFS of the equivalence ratio and of the dilution. At very lean condition it slightly overestimates the value. At rich conditions the almost asymptotic behavior is globally reconstructed, but an oscillatory shape, probably induced by the quadratic terms in (5), must be noted.

3.3. LFS at engine-like conditions

In the following figures pressure, temperature and diluent effects on LFS are shown. In order to optimize the space in each figure, the minimum ($p = 50$ bar) and maximum ($p = 290$ bar) pressures of the space are indicated with p-Lo and p-Hi respectively, and the same for the minimum ($T = 400$ K) and maximum ($T = 700$ K) temperatures are referred to as T-Lo and T-Hi, respectively.

3.3.1. Effect of pressure and temperature

As one can see in figure 3, an increase in the mixture temperature leads to an increase in LFS irrespective of the equivalence ratio. At lean (figure 3a) and stoichiometric (figure 3b) conditions, a pressure increase produces a reduction of LFS. These results are confirmed by the experimental evidence even if obtained at lower pressure and temperature values. At mixture rich condition (figure 3c) this effect is reversed: a pressure increase produces an increase of the LFS. It is also evident that at rich conditions the flame is still able to sustain itself.

3.3.2. Analytic correlation for engine-like space

Figure 4a, in which each curve has been normalized against its maximum value, shows that the equivalence ratio for the maximum laminar velocity and the dependency between LFS and the equivalence ratio for lean to stoichometric mixture is independent from the thermodynamic conditions on the mixture. This indicated that using a constant value for α and β exponents in equation (1) can be a viable solution. But a constant, being a simple scaling factor, will be not able to reproduce the asymmetry that the φ-S_L correlation shows for rich to very-rich conditions (again see figure 4a). The power exponent in the form of the equation (3) has been unsuccessfully applied (figure 4b), since the power law amplifies the previously observed oscillation at rich and very rich condition toward non-physical values.
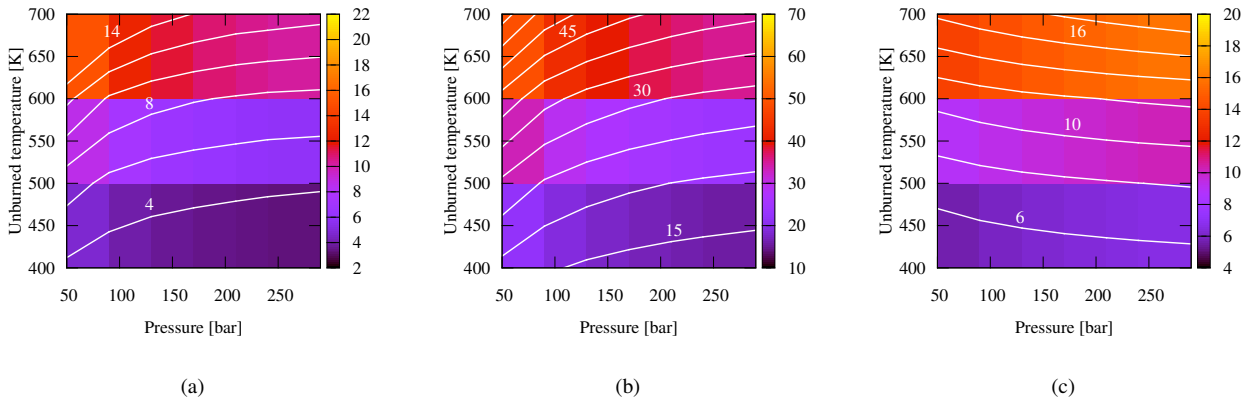
Figure 3: Combined effect of pressure and temperature on TAE's LFS, undiluted mixture. Planes at constant equivalence ratio: (a) $\varphi = 0.6$ (b) $\varphi = 1.0$ (c) $\varphi = 2.4$

Using `T-Lo-p-Lo` thermodynamic mixture value as the reference condition for $S_{L,0}$, somehow reduces the oscillation (figure 4c). So it can be stated that a correlation in the form of (1) is not really applicable to the engine-like undiluted space and the linear interrogation of the tabulated engine-like space must be preferred.

3.3.3. Effect of the dilution with EGR and water

As can be see from figure 5a (for `T-Hi` and `p-Hi` conditions, the observation remains valid for the other points of the engine space) increasing the amount of diluents, for a given equivalence ratio, leads to a progressive reduction, as expected, of the LFS, reduction that becomes less and less sensitive to diluent mass fraction as the equivalence ratio increases. The same effect can be seen observing the relative reduction effect of pure water (figure 5b) and pure EGR (figure 5c), for a given thermodynamic condition: the increase of diluent quantity reduces the LFS. The effect is almost linear when the diluent mass fraction is small, as can be seen for water in figure 5b. The effect loses linearity when high mass fraction are involved (figure 5c when $x_{egr} \geq .1$). In figures 5b and 5c can also be observed that for a given mass fraction, the reduction effect decreases as the temperature of the initial mixture (unburned temperature) increases, whereas the pressure has an almost non existent effect.

The combined effect of EGR and water (restricted to the knock-prevention space) is almost linear in both mass fractions and doesn't show a cross interaction (figure 6a). In order to better asses its effect, the LFS values obtained
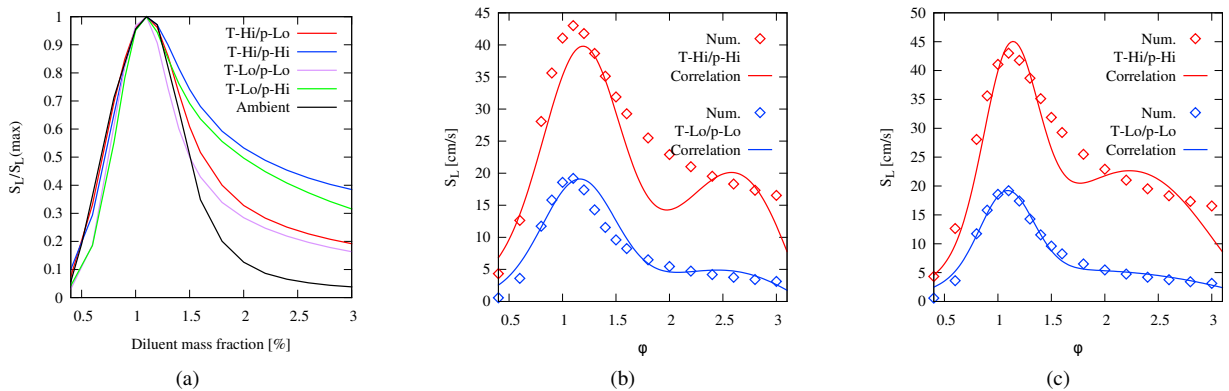

Figure 4: TAE's LFS at different engine-like thermophysical conditions, undiluited mixture. (a) Relative effect. Analitycal correlation: (b) using the ambient reference condition. (c) using `T-Lo` and `p-Lo` as reference condition.
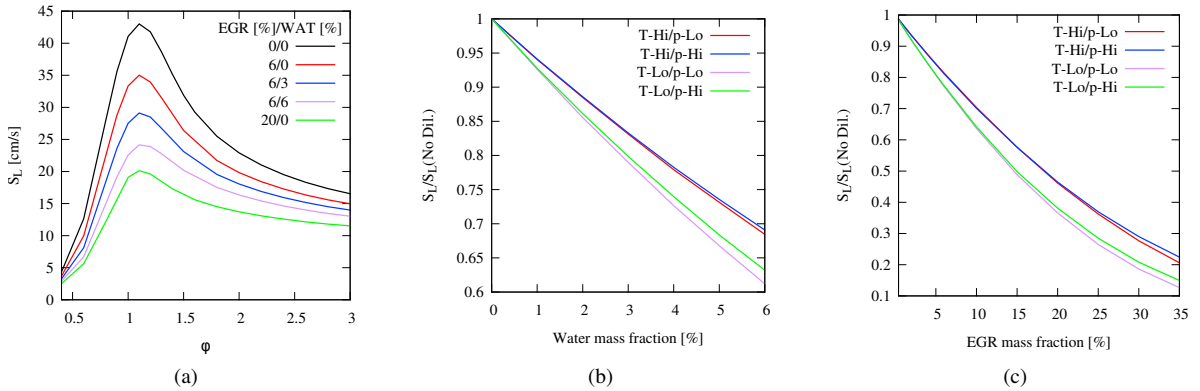
Figure 5: Effect of EGR and water dilution on TAE's LFS. (a) `T-Hi`, `p-Hi` thermodinamic condition. Relative effect of pure diluent at different thermodinamic conditions and $\varphi = 1$: (b) pure water (c) pure EGR

for the `T-Hi` and `p-Hi` thermodynamic conditions and keeping the total mass fraction of diluent constant ($x_{EGR}+x_{wat} = 0.06$) are reported in figure 6 for lean, stoichometric and rich conditions. As one can observe, the LFS is higher for stoichometric conditions and the previously observed asymmetry between rich and lean conditions is not affected by the diluition. It must be noted that for each condition the maximum value is obtained with a pure water diluition. The water effect is highlighted in figure 6b were the LFS has been normalized against the maximum value for each conditions: all the curves reach the maximum with zero water. It must also be noted that the relative reduction effect is almost the same between lean and stoichometric conditions, almost non existant for rich condition.

4. Conclusion

A previously implemented numerical methodology, based on an open source mono-dimensional adiabatic laminar flame solver and a literature chemical kinetics mechanism, has been extend in order to account for the combined effect of two different mixture diluents on the LFS of a generic fuel. The resulting code has been applied to the evaluation of the LFS of a gasoline surrogate, representative of a commercial gasoline, on a multidimensional space of equivalence ratio, pressure, temperature value variable in a range typical of a GDI SI engine. The added EGR and water masses as diluents are in the range of a knock-prevention strategy.
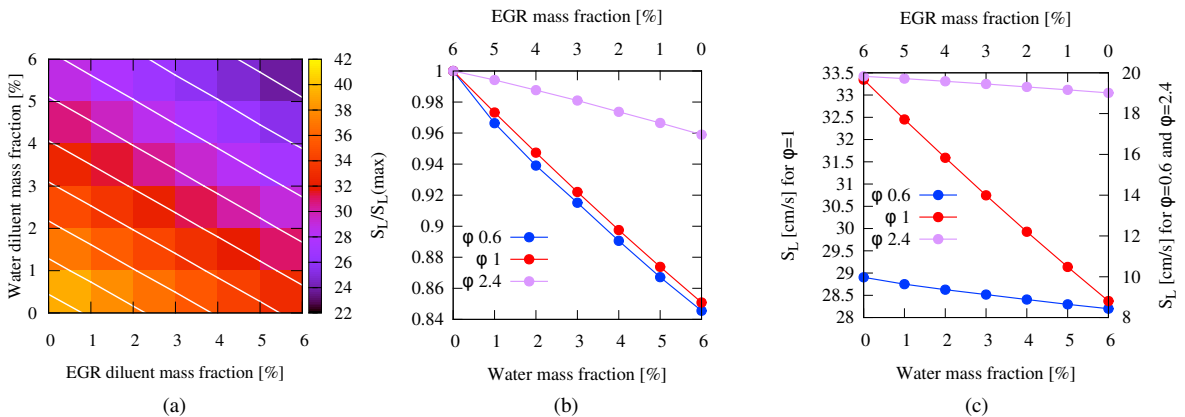

Figure 6: Combined effect of EGR and water diluition on TAE's LFS, thermophysical condtions: `T-Hi` and `p-Hi`. (a) plane with $\varphi = 1$. (b) LFS with constant total mass fraction of diluent (c) Relative LFS with constant total mass fraction of diluent

Using the numerical result, a correlation accounting for the effect of φ, EGR and water has be defined at ambient pressure and temperature values. The same correlation cannot be extended with a literature-standard power-law correction to engine-like conditions due to some nonlinear cross-effects between pressure and temperature that produce oscillatory and unphisycal values for the LFS. Increasing the unburned temperature increase the LFS value, as expected. The pressure increase reduces the LFS value only in the range from lean to stoichometric conditions; at very rich conditions, the effect is reversed. Moreover at engine-like thermodynamic rich conditions the flame is capable of sustain itself.

In agreement with the findings from the literature, adding a quantity of diluent causes a reduction of the LFS. This reduction is substantially linear if the added mass fraction is limited to low values; at high values, the effect is almost parabolic. The quality of the diluent is also of paramount importance: it must be noted that at engine-like pressure and temperature conditions, if the total diluent mass fraction is kept constant, the reducing effect of pure water is greater than the one of pure EGR.

References

[1] Peters, N.. Turbulent Combustion. Cambridge Monographs on Mechanics; 1 ed.; Cambridge: Cambridge University Press; 2000. ISBN 9780521660822,0521660823. doi:10.1017/CBO9780511612701.

[2] Ladommatos, N., Abdelhalim, S., Zhao, H.. The effects of exhaust gas recirculation on diesel combustion and emissions. International Journal of Engine Research 2000;1(1):107–126. doi:10.1243/1468087001545290.

[3] Bianchi, G., Cazzoli, G., Pelloni, P., Corcione, F.. Numerical study towards smoke-less and nox-less hsdi diesel engine combustion. SAE Technical Papers 2002;doi:10.4271/2002-01-1115.

[4] Dryer, F.. Water addition to practical combustion systems-concepts and applications. Symposium (International) on Combustion 1977;16(1):279–295. doi:10.1016/S0082-0784(77)80332-9.

[5] Kohketsu, S., Mori, K., Sakai, K., Nakagawa, H.. Reduction of exhaust emission with new water injection system in a diesel engine. SAE Technical Papers 1996;doi:10.4271/960033.

[6] D'Adamo, A., Berni, F., Breda, S., Lugli, M., Fontanesi, S., Cantore, G.. A numerical investigation on the potentials of water injection as a fuel efficiency enhancer in highly downsized gdi engines. SAE Technical Papers 2015;2015-April(April). doi:10.4271/2015-01-0393.

[7] Cavina, N., Rojo, N., Businaro, A., Brusa, A., Corti, E., De Cesare, M.. Investigation of water injection effects on combustion characteristics of a gdi tc engine. SAE International Journal of Engines 2017;10(4). doi:10.4271/2017-24-0052.

[8] Rallis, C., Garforth, A.. The determination of laminar burning velocity. Progress in Energy and Combustion Science 1980;6(4):303–329. doi:10.1016/0360-1285(80)90008-8.

[9] Kumar, K., Sung, C.J.. Laminar flame speeds and extinction limits of preheated n-decane/o2/n2 and n-dodecane/o2/n2 mixtures. Combustion and Flame 2007;151(1-2):209–224. doi:10.1016/j.combustflame.2007.05.002.

[10] Jerzembeck, S., Peters, N., Pepiot-Desjardins, P., Pitsch, H.. Laminar burning velocities at high pressure for primary reference fuels and gasoline: Experimental and numerical investigation. Combustion and Flame 2009;156(2):292–301. doi:10.1016/j.combustflame.2008.11.009.

[11] Gilbert, M.. The influence of pressure on flame speed. Symposium (International) on Combustion 1957;6(1):74–83. doi:10.1016/S0082-0784(57)80013-7.

[12] Metghalchi, M., Keck, J.. Burning velocities of mixtures of air with methanol, isooctane, and indolene at high pressure and temperature. Combustion and Flame 1982;48(C):191–210. doi:10.1016/0010-2180(82)90127-4.

[13] Cazzoli, G., Forte, C., Bianchi, G., Falfari, S., Negro, S.. A chemical-kinetic approach to the definition of the laminar flame speed for the simulation of the combustion of spark-ignition engines. SAE Technical Papers 2017;2017-September. doi:10.4271/2017-24-0035.

[14] Falfari, S., Bianchi, G., Cazzoli, G., Forte, C., Negro, S.. Basics on water injection process for gasoline engines; 2018.

[15] Goodwin, D.G., Moffat, H.K., Speth, R.L.. Cantera: An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes. http://www.cantera.org; 2016. doi:10.5281/zenodo.170284.

[16] Mazas, A., Fiorina, B., Lacoste, D., Schuller, T.. Effects of water vapor addition on the laminar burning velocity of oxygen-enriched methane flames. Combustion and Flame 2011;158(12):2428–2440. doi:10.1016/j.combustflame.2011.05.014.

[17] Smith, G.P., Golden David, M., Frenklach, M., Moriarty, N.W., Eiteneer, B., Goldenberg, M., et al. GRI-Mech 3.0. 2000. URL: http://www.me.berkeley.edu/gri_mech/.

[18] Ranzi, E., Frassoldati, A., Grana, R., Cuoci, A., Faravelli, T., Kelley, A., et al. Hierarchical and comparative kinetic modeling of laminar flame speeds of hydrocarbon and oxygenated fuels. Progress in Energy and Combustion Science 2012;38(4):468–501. doi:10.1016/j.pecs.2012.03.004.

[19] Dirrenberger, P., Glaude, P., Bounaceur, R., Le Gall, H., Da Cruz, A., Konnov, A., et al. Laminar burning velocity of gasolines with addition of ethanol. Fuel 2014;115:162–169. doi:10.1016/j.fuel.2013.07.015.

[20] Galmiche, B., Halter, F., Foucher, F.. Effects of high pressure, high temperature and dilution on laminar burning velocities and markstein lengths of iso-octane/air mixtures. Combustion and Flame 2012;159(11):3286–3299. doi:10.1016/j.combustflame.2012.06.008.