

Full Length Article

A correlation to compute the thermo-diffusive instability effect of lean hydrogen flames at engine-like conditions

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ABSTRACT

Lean hydrogen mixtures are a valid alternative to conventional fuels for internal combustion engine. Lean hydrogen flames are characterised by a low effective Lewis number, which triggers flame instabilities. Therefore, being able to correctly quantify the effect of such phenomenon on the flame propagation is important. However, the computation of the flame instability second order growth rate (ω_2), which is widely used to model the laminar flame speed increase due to instabilities, is not straightforward, as chemical kinetics must be considered. In this work, a comprehensive correlation for modelling thermo-diffusive instabilities at engine-like conditions is presented, and an easy-to-implement correlation for the enhancement of the flame speed is proposed. As a first step, one-dimensional freely propagating flame simulations are used to compute the thermal expansion parameter σ of lean hydrogen flames. Secondly, by imposing the Sutherland's Law to describe the mixture thermal conductivity, the terms that include the stabilising (or destabilising) effects of heat diffusion (B_1), molecular diffusion (B_2), and viscous diffusion (B_3) are computed, and a fitting function is found for each of them. Thirdly, the computation of the Zel'dovich number β is performed, and a fitting procedure carried out. Finally, by the resulting fitting functions, an ω_2 correlation dependent only on the local thermodynamic conditions of the mixture is developed within pressure, unburnt temperature and equivalence ratio ranges of 10–50 bar, 500–900 K and 0.2–0.7, respectively. Furthermore, reasonable results can be found through extrapolation up to 100 bar and 1100 K. The flame speed enhancement values obtained with the developed correlation differ by less than 6% from those reported in literature at relevant light-duty engine-like conditions. Larger discrepancies are observed only at low unburnt gas temperatures (300 K) or for very lean mixtures ($\Phi = 0.2$).

1. Introduction

There is a growing interest in hydrogen to reduce the carbon footprint of human activities [1]. Along with Battery Electric Vehicles (BEVs), hydrogen can be one of the feasible options to progressively decarbonize the transport sector through hydrogen-fuelled internal combustion engines (H2ICEs) [2] and Fuel-Cells Electric Vehicles (FCEVs) [3].

As for the former, several works show that the strategy for highest efficiency is represented by lean-hydrogen mixtures. In fact, given the high laminar flame speed and the broad flammability range of hydrogen, comparable burn rates can be obtained with respect to engines operated with carbon-based fuels [4] when lean hydrogen mixtures are utilised. Despite this promising characteristic, engine power output must be carefully evaluated, since the low H_2 density negatively impacts the volume-based energy content [5]. Therefore, high-pressure direct

injection is usually required to run high-power density engines, increasing complexity and cost of this technology.

The flame propagation of lean H_2 mixtures is affected not only by hydrodynamic instability, which is caused by the density jump across the flame front [6,7], but also by the thermo-diffusive one. This phenomenon is driven by the lower-than-unity Lewis number, defined as the ratio between thermal and mass diffusivity of the mixture. Indeed, hydrogen is characterized by a higher mass diffusivity if compared to conventional fuels [8], which leads to the amplification of the perturbations and to the enhancement of the flame front wrinkling. For instance, if the reaction zone is convex towards the unburnt mixture, it cools down more slowly than it is enriched by additional supply of fresh fuel, which locally increases the equivalence ratio and, consequently, the flame speed. Vice versa, when the reaction zone is convex to the burnt mixture, the temperature increase is slower than the fuel depletion, resulting in a further decrease of the flame speed [9].

Theoretical studies were conducted to quantify the effect of

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Nomenclature

σ	Thermal expansion parameter
ρ_u	Unburnt density
ρ_b	Burnt density
S_L	Unstretched Laminar Flame Speed
S_M	Enhanced Laminar Flame Speed
ω_2	Second Order Instability Parameter
Le_{eff}	Effective Lewis number
Pr	Prandtl number
p	Pressure
Φ	Equivalence Ratio
T_u	Unburnt Temperature
T_b	Burnt Temperature
δ_L	Laminar Flame Thickness
CFD	Computational Fluid Dynamics
λ	Thermal Conductivity
$\tilde{\lambda}$	Normalised Thermal Conductivity
x	Normalised Temperature
E_a	Activation Energy

instabilities. By considering the density jump on the flame front, an unbounded increase of the growth rate with the wavelength, which is not observed experimentally, is found [6,7]. Matalon et al. [10], Frenkel et al. [11], and Pelce et al. [12] all proved that by including differential diffusion effects through a second order term in the dispersion function, a stabilization effect at large wavenumber can be achieved. Several studies can be found in literature where the experimental investigation of such phenomenon is performed. Xie et al. [13] analysed the impact of pressure (from 0.1 to 0.5 MPa), temperature (from 300 K to 400 K), and equivalence ratio (from 0.4 to 1.5) on the onset of cellular structures on a hydrogen premixed flame propagating in a fan-stirred vessel, and a few parameters, such as the critical flame radius, Peclet number, Markstein number, and Karlovitz number, are analysed to be able to predict the flame behaviour. Xu et al. [14] examined the effect of increasing pressure (from 2 bar to 3 bar), initial temperature (from 298 K to 428 K) and hydrogen addition (from 40% to 50%) on the cellularity of spherically expanding ammonia/hydrogen blends flames in a constant volume vessel. Both these works show increasing cellular structures with increasing pressure, decreasing temperature and with leaner hydrogen mixtures. In contrast, for ammonia blends, the mixture with the highest H_2 concentration is the most susceptible to instability. These trends can be noted also in numerical investigations through DNS simulations, as shown in the work of Berger et al. [15], where variations of pressure, equivalence ratio and temperature are performed in a two-dimensional domain, where a weak harmonic perturbation is applied on a freely-propagating flame, and the growth rate is analysed. Particularly, in this work, the authors introduce a fourth-order term in the dispersion relation, as in [9]. Howarth et al. [16] developed an empirical model that links the second order parameter and the enhanced flame speed through two-dimensional DNS simulations, and analyses on freely propagating flames in a three-dimensional domain confirmed that the same functions can be used with a slight correction on the model constants [17].

In ICEs, despite the high pressure reached in the combustion chamber due to compression, experimental observation of flame instabilities onset is more difficult for two main reasons. Firstly, the high unburnt temperatures reached at the end of the compression stroke reduce the thermo-diffusive instability impact on the flame development. Secondly, the unburnt mixture is not quiescent, and the flame wrinkling effect due to turbulence is predominant. For instance, Ye et al. [18] deployed laser-induced fluorescence of a tracer to detect flame corrugation in an optically accessible hydrogen-fuelled engine revving at 400 rpm and 800

rpm and with an equivalence ratio of 0.4. Results show a marked cellular structures growth at 400 rpm, while turbulence disrupts thermo-diffusive cell formation at 800 rpm. Nevertheless, authors suggest that flame instabilities should be taken into account in numerical framework, as they still play a major role in flame dynamics and they may affect the early stages of flame propagation. This is also supported by the work of Chu et al. [19], where the authors performed DNS analyses of $\Phi = 0.4$ hydrogen flame kernel development at 40 bar and 800 K. Results show that differential diffusion increases the flame stretch factor by more than four times if compared to the value obtained without thermo-diffusive instability, which indicates that this phenomenon may affect the combustion development also at engine-like conditions. In engine simulations, different approaches were considered to account for thermo-diffusive instability effect on flame propagation. Ramognino et al. [20] adopted the correlation proposed in [15] to increase the unstretched laminar flame speed value when instabilities are triggered, while Scalambro et al. [21] replicated the methodology proposed in [17], and the enhanced flame speed due to thermo-diffusive instability onset was tabulated and used in the CFD framework. The same strategy was adopted by Sfriso et al. [22] and Hernandez et al. [23].

All previously proposed approaches require the tabulation of a correction factor to account for the amplification of the flame speed due to instabilities. However, these tables are typically not provided in the literature, which introduces significant uncertainties when attempting to implement a tabulated approach. Incorporating the effects of thermo-diffusive instabilities within a CFD framework (e.g., following [17]) currently requires multiple offline preprocessing steps, including detailed chemical kinetics calculations. These requirements make the model's independent reproduction non-trivial and highly sensitive to user choices, such as mechanism selection and activation-energy evaluation methodology. The objective of this work is to apply the approach proposed in [17] and to develop a novel and easy-to-implement correlation that can be used independently of the CFD code or the combustion model used.

2. Theoretical background

A premixed flame propagating into a quiescent fresh mixture is affected by intrinsic instabilities, which are governed by two main phenomena. The density jump across the flame promotes the hydrodynamic or Darrieus-Landau (DL) instability [6,7]. The difference between mass and thermal diffusivities of the deficient and dominant reactants determines the onset of the thermo-diffusive instability. By considering a flame sheet of the form (Eq. (1)), where A is the amplitude of the perturbation, the normalised growth rate $\tilde{\omega}$, defined as (Eq. (2)), where δ_L is the flame thickness and S_L the laminar flame speed, can be described by Eq. (3), where σ is the thermal expansion ratio, i.e. the ratio between the unburnt and burnt density. $\tilde{k}$ is the normalised wavelength of the perturbation.

$$F(x, t) = A e^{i k x + \omega t} \quad (1)$$

$$\tilde{\omega} = \omega \delta_L / S_L \quad (2)$$

$$\tilde{\omega} = \frac{1}{\sigma + 1} \left(\sqrt{\sigma^3 + \sigma^2 - \sigma} - \sigma \right) \tilde{k} = \omega_{DL} \tilde{k} \quad (3)$$

As previously described, an unbounded perturbation growth with the wavelength is predicted, which is not observed in experiments. By including the thermal and mass diffusion effects by a second order term that solves the unboundedness problem, a new formulation of $\tilde{\omega}$ can be written, as shown in Eq. (4) [10–12], where ω_2 is the second order instability parameter, which can be written in the general form of Eq. (5). Pr is the Prandtl number, while B_1 , B_2 , and B_3 Eq. (6), Eq. (7) and Eq. (8) represent the stabilizing or destabilizing effects of thermal, mass and viscous diffusion, respectively. β is the Zel'dovich number.

$$\tilde{\omega} = \omega_{DL}\tilde{k} + \omega_2\tilde{k}^2 \quad (4)$$

$$\omega_2 = -[B_1 + \beta(\text{Le}_{\text{eff}} - 1)B_2 + \text{Pr}B_3] \quad (5)$$

$$B_1 = \frac{\sigma}{(2(\sigma + (\sigma + 1)\omega_{DL}))} \left(\frac{\sigma(2\omega_{DL} + \sigma + 1)}{\sigma - 1} \int_1^{\sigma} \frac{\tilde{\lambda}(x)}{x} dx + \int_1^{\sigma} \tilde{\lambda}(x) dx \right) \quad (6)$$

$$B_2 = \frac{\sigma(1 + \omega_{DL})(\sigma + \omega_{DL})}{2(\sigma - 1)(\sigma + (\sigma + 1)\omega_{DL})} \int_1^{\sigma} \log\left(\frac{\sigma - 1}{x - 1}\right) \frac{\tilde{\lambda}(x)}{x} dx \quad (7)$$

$$B_3 = \frac{\sigma}{\sigma + (\sigma + 1)\omega_{DL}} \left((\sigma - 1)\tilde{\lambda}(\sigma) - \int_1^{\sigma} \tilde{\lambda}(x) dx \right) \quad (8)$$

In the formulation of B_i , $\tilde{\lambda}$ and x are the thermal conductivity and temperature, respectively, both normalized by their unburnt mixture values. As for β , it is calculated through Eq. (9) and it includes the activation energy of the mixture. As suggested in [24], it can be computed by performing the derivative of $\log(\rho_u S_L)$ over $1/T_b$ Eq. (10) for each condition.

$$\beta = \frac{E_a}{R} \frac{T_b - T_u}{T_b^2} = -2\alpha \frac{T_b - T_u}{T_b^2} \quad (9)$$

$$\alpha = \frac{d(\log(\rho_u S_L))}{d(1/T_b)} \quad (10)$$

Once β is computed, the effective Lewis number of the mixture Le_{eff} can be calculated as in Eq. (11), where Le_O and Le_F are the Lewis numbers of oxidizer and fuel, both computed as the thermal diffusivity of the mixture over the mass diffusivity of the respective reactant.

$$\text{Le}_{\text{eff}} = \begin{cases} \frac{\text{Le}_O + A\text{Le}_F}{1 + A} \text{ with } A = 1 + \beta(\Phi^{-1} - 1) \text{ if } \Phi < 1 \\ \frac{\text{Le}_F + A\text{Le}_O}{1 + A} \text{ with } A = 1 + \beta(\Phi - 1) \text{ if } \Phi > 1 \end{cases} \quad (11)$$

Once the second order parameter is calculated, the model proposed in [17] can be adopted. Particularly, the ratio between the flame speed affected by the instabilities (S_M) and the unstretched value is shown in Eq. (12).

$$\frac{S_M}{S_L} = \begin{cases} \exp(0.08 \omega_2) \text{ with } p < p_c \\ 1 + 0.47 \omega_2 \text{ with } p \geq p_c \end{cases} \quad (12)$$

The critical pressure p_c , which divides the ω_2 space in high and low pressure zone, is the value above which, for a given Φ , the activation energy decreases due to the release of reactive H and OH radicals [25]. This threshold can be described through the empirical expression Eq. (13), where p_{ref} is the reference pressure set to 1 atm, and Θ is the ratio between mixture and reference temperatures, with the second one set to 300 K.

$$p_c = p_{\text{ref}} \left(\frac{20\Phi}{7 - 2\Theta} \right)^{\frac{150}{21+10\Theta}} \quad (13)$$

3. Methodology and results

The online computation of ω_2 is not trivial, especially in a multi-dimensional CFD framework. The idea of the proposed methodology is to obtain an algebraic correlation to compute the second-order instability parameter through a function solely dependent on the thermodynamic conditions of the mixture, applying the model proposed in [17]. To do so, chemical kinetics simulations are adopted and carried out with the software DARS, licensed by Siemens DISW, while data

analysis and fitting procedures are performed through MATLAB scripts.

3.1. Computation and fitting of σ and B_i

The first step is the computation of σ . To this end, a freely propagating flame is adopted, and a range of engine-like thermodynamic conditions is considered, i.e. unburnt temperature from 700 to 1200 K, pressures from 5 to 50 bar and equivalence ratio from 0.2 to 1.2. Coherently with [17] the Burke mechanism [26] is used for this analysis. The graph in Fig. 1a shows the resulting σ values over the equivalence ratio of the mixture, at different pressure and temperature levels. It is notable that the thermal expansion has a strong dependence on both Φ and T_u , while a minor variation with pressure is visible. The most relevant pressure dependency can be seen with nearly stoichiometric mixtures and unburnt temperatures higher than 1000 K. However, with such conditions, the thermo-diffusive effect on hydrogen flame can be neglected.

A fitting procedure of the results obtained at 20 bar is then considered, and a quadratic function of Φ is found for each T_u (Eq. (14)). The C term of Eq. (14) is constant, while both A and B can be described by a second order polynomial function of T_u . Fig. 1b depicts the value of the coefficients of Eq. (14) for each T_u (scatter plots), along with their respective fitting functions (Eq. (15), Eq. (16), and Eq. (17)). Therefore, $\sigma_{\text{fit}}(\Phi, T_u)$ has a quadratic dependence on both the equivalence ratio and unburnt temperature.

$$\sigma_{\text{fit}}(\Phi, T_u) = A(T_u) \Phi^2 + B(T_u) \Phi + C \quad (14)$$

$$A(T_u) = a_1 T_u^2 + a_2 T_u + a_3 \quad (15)$$

$$B(T_u) = a_4 T_u^2 + a_5 T_u + a_6 \quad (16)$$

$$C = a_7 \quad (17)$$

The a_i coefficients can be found in Appendix A.

To compute the B_i terms, it is necessary to calculate ω_{DL} , which is straightforward once σ is known (Eq. (3)), and the three integrals that can be seen in Eq. (6), Eq. (7) and Eq. (8).

In this work, to be consistent with the CFD methodology proposed by the authors [27], Sutherland's law (Eq. (18)) is used to compute the thermal conductivity, and given the higher mass percentage of nitrogen in each mixture, the coefficients λ_0 , T_0 and S used for N_2 are set.

$$\frac{\lambda}{\lambda_0} = \left(\frac{T}{T_0} \right)^{3/2} \left(\frac{T_0 + S}{T + S} \right) \quad (18)$$

Therefore, it is possible to analytically calculate the integrals. As shown, the pressure value does not affect $\lambda(x)$, hence, B_i can be calculated only by considering equivalence ratio and temperature of the mixture. Fig. 2 shows the results of B_i as a function of the unburnt temperature of the mixture, for different values of the thermal expansion ratio, ranging from 1.5 to 3.5. These values cover a broad range of conditions, as it can be noted in Fig. 1.

Given these profiles, a second order polynomial function of the unburnt temperature is the best fitting function to compute the B_i terms, as reported in Eq. (19), Eq. (20), and Eq. (21).

$$B_1(\sigma, T_u) = D(\sigma) T_u^2 + E(\sigma) T_u + F(\sigma) \quad (19)$$

$$B_2(\sigma, T_u) = G(\sigma) T_u^2 + H(\sigma) T_u + I(\sigma) \quad (20)$$

$$B_3(\sigma, T_u) = J(\sigma) T_u^2 + K(\sigma) T_u + L(\sigma) \quad (21)$$

To account for the σ dependency, a fitting procedure is considered for the coefficients of B_i . A second order polynomial function is found to well reproduce the behaviour of each coefficient (Eqs. (22)–(30)), and the values of b_i can be found in Appendix A.

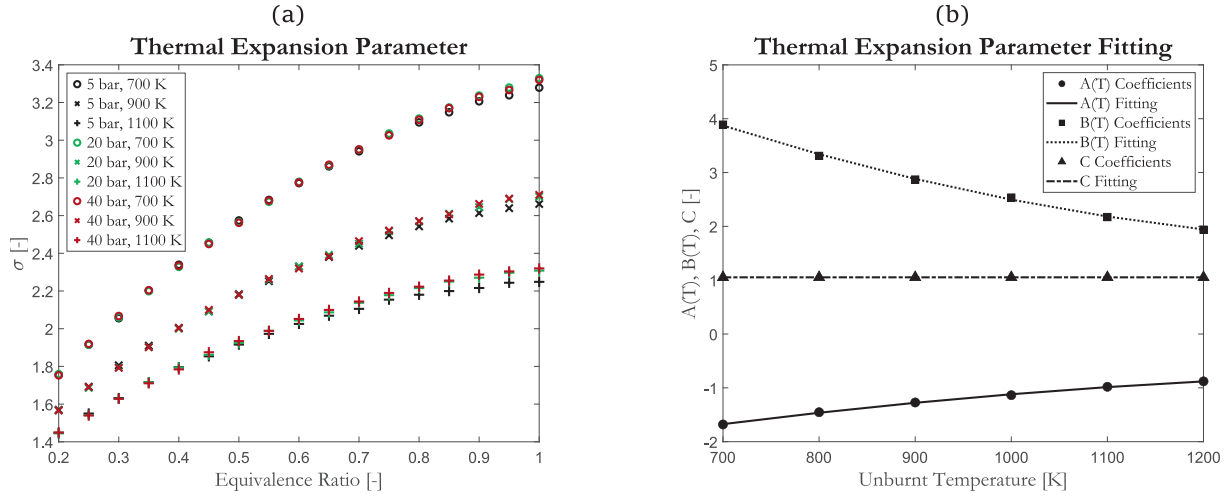


Fig. 1. (a) Thermal expansion parameter for hydrogen mixtures with $0.2 \leq \Phi \leq 1.0$ at 5 bar (black), 20 bar (green), and 40 bar (red), and with temperatures of 700 K (circle), 800 K (cross), and 900 K (plus). (b) Second order (circle), first order (square), and constant (triangles) parameters of the fitting function, at each temperature. The fitting function of second order (solid line), first order (dotted line), and constant (dashed dotted line) parameters are reported. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

$$D(\sigma) = b_1 \sigma^2 + b_2 \sigma + b_3 \quad (22)$$

$$E(\sigma) = b_4 \sigma^2 + b_5 \sigma + b_6 \quad (23)$$

$$F(\sigma) = b_7 \sigma^2 + b_8 \sigma + b_9 \quad (24)$$

$$G(\sigma) = b_{10} \sigma^2 + b_{11} \sigma + b_{12} \quad (25)$$

$$H(\sigma) = b_{13} \sigma^2 + b_{14} \sigma + b_{15} \quad (26)$$

$$I(\sigma) = b_{16} \sigma^2 + b_{17} \sigma + b_{18} \quad (27)$$

$$J(\sigma) = b_{19} \sigma^2 + b_{20} \sigma + b_{21} \quad (28)$$

$$K(\sigma) = b_{22} \sigma^2 + b_{23} \sigma + b_{24} \quad (29)$$

$$L(\sigma) = b_{25} \sigma^2 + b_{26} \sigma + b_{27} \quad (30)$$

Fig. 3 depicts the comparison between each function that describes the coefficients of B_i with their respective raw values, for each σ . Results show a perfect agreement over the whole range analysed. The lowest coefficient of determination (R^2) (determined as in Eq. (31), where X indicates the generic coefficient of B_i) is for $J(\sigma)$ and it is equal to 99.9045%, proving the robustness of the methodology.

$$R^2 = 1 - \frac{(X_{\text{predicted}} - X_{\text{actual}})^2}{(X_{\text{predicted}} - X_{\text{mean}})^2} \quad (31)$$

3.2. Computation and fitting of β

As described in Section 2, the Zel'dovich number β requires an additional step, as the laminar flame speed computation is necessary to define the mixture activation energy. Firstly, a chemical mechanism sensitivity is performed. Along with the Burke scheme already used for the previous analyses, the ones proposed by Konnov [28], Ó Conaire et al. [29], and Ranzi et al. [30–32] are tested.

Fig. 4 shows the unstretched laminar flame speed obtained with each mechanism at 5 bar and 25 bar, at 700 K, 800 K, and 900 K, and with $0.2 \leq \Phi \leq 0.7$. The overall behaviour of each mechanism is similar. At 5 bar, the CRECK mechanism results in a slightly higher unstretched laminar flame speed at every temperature considered, while at 25 bar the highest laminar flame speed is obtained with Burke.

Given the similar unstretched laminar flame speed values obtained with different mechanisms, α , defined as in Eq. (10), is also expected to have comparable values when computed with different chemical definitions. The computation of α is not trivial. It involves, for each thermodynamic condition, the calculation of the derivative of the product between laminar flame speed and unburnt density with respect to the inverse of the burnt gas temperature, without changing pressure, temperature and equivalence ratio. This can be performed by either adding a small amount of N_2 , as suggested by Sun et al. [33] and performed in [15], or by substituting a small amount of nitrogen in the definition of the oxidizer with the same amount of argon, as suggested in [24] and performed in [17]. Particularly, in this last work, the authors show that by considering increasing amounts of argon up to 0.2 mol in a hydrogen mixture at 5 atm, 300 K and equivalence ratio of 0.38, a linear fit can be found that describes the behaviour of $\log(\rho_u S_L)$ against $1/T_b$. Thereby, at the analysed condition, the resulting activation energy, and thus ω_2 , should be independent from the chosen amount of argon. To better understand the effect of each strategy adopted to compute α , both the approaches are here tested, and the Burke mechanism is used for these sensitivities.

Fig. 5a depicts the $\log(\rho_u S_L)$ over $1/T_b$ trend at the same thermodynamic conditions considered in [17], and, as a reference, the results in [17] have been extrapolated and reported here (square symbol), along with the best linear fit found in that work (black solid line). The reference state, i.e. the one without the argon substitution or nitrogen addition, is reported with a black filled dot. A good agreement is found with the literature data, as this point lays on the linear fit.

By considering 0.1 and 0.2 mol of argon, the blue filled dots are obtained, and a linear interpolating function is calculated for both argon amounts starting from the reference state. The same trend of [17] is found here. Indeed, the two linear coefficients computed are $-2.751e+04$ with 0.1 mol and $-2.714e+04$ with 0.2 mol, which lead to a negligible difference in terms of ω_2 value at this specific thermodynamic condition. However, since these points are not perfectly aligned with the literature fitting function, the computed gradients differ, and this behaviour might be related to the different chemistry solver used.

The second approach based on additional N_2 is also tested. Particularly, the mole fraction of N_2 is increased, up to 20%. The green scatter plot in Fig. 5b depicts the results of this sensitivity, with a 2% interval. Results show that up to 10% of additional N_2 , a linear dependence can be noted, as the scatter plots lay on the green dashed-dotted line, which is obtained by interpolating the reference state value and the 5% one. The

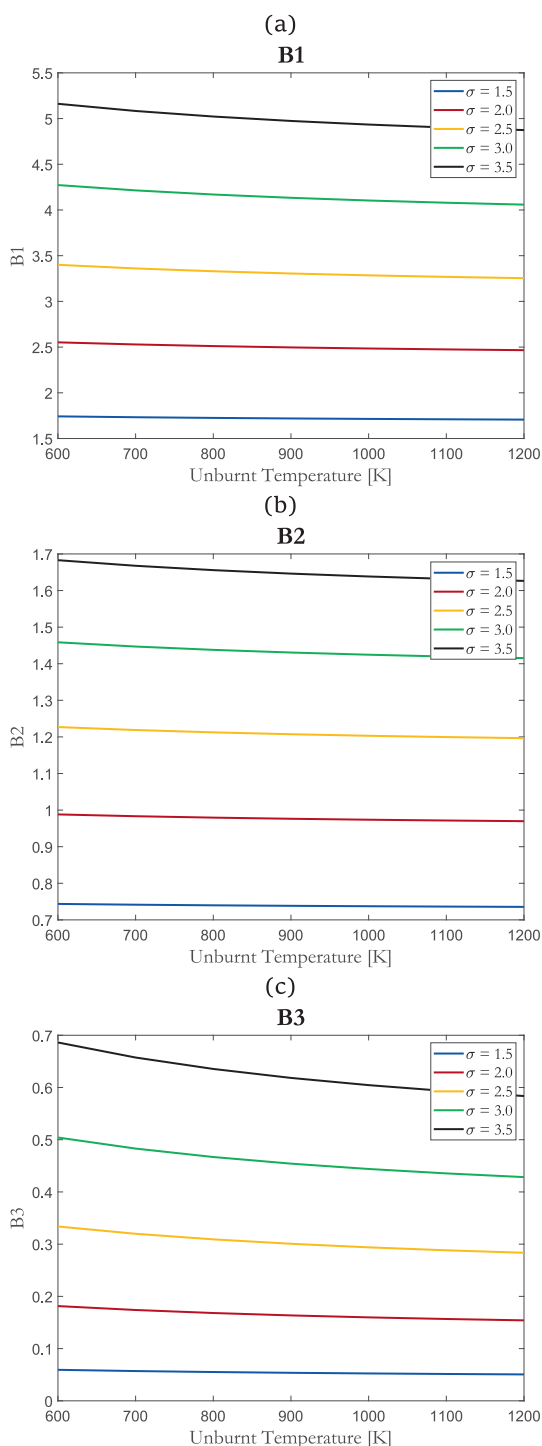


Fig. 2. Resulting B_1 (a), B_2 (b), and B_3 (c), for $600 \text{ K} \leq T \leq 1200 \text{ K}$, with σ set to 1.5 (blue), 2.0 (red), 2.5 (yellow), 3.0 (green), and 3.5 (black). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

resulting gradient is only 7% lower than the one observed with 0.2 mol of argon, indicating that the same gradient can be found regardless the adopted approach. With higher concentrations of N_2 , data start to deviate from this line. With a 20% addition, the resulting α is in good agreement with the one found in the literature, as the green solid line is almost superimposed to the one found through a linear fitting of the literature data. Therefore, a ω_2 closer to the one obtained in [17] can be obtained at this specific thermodynamic condition, even though a 20%

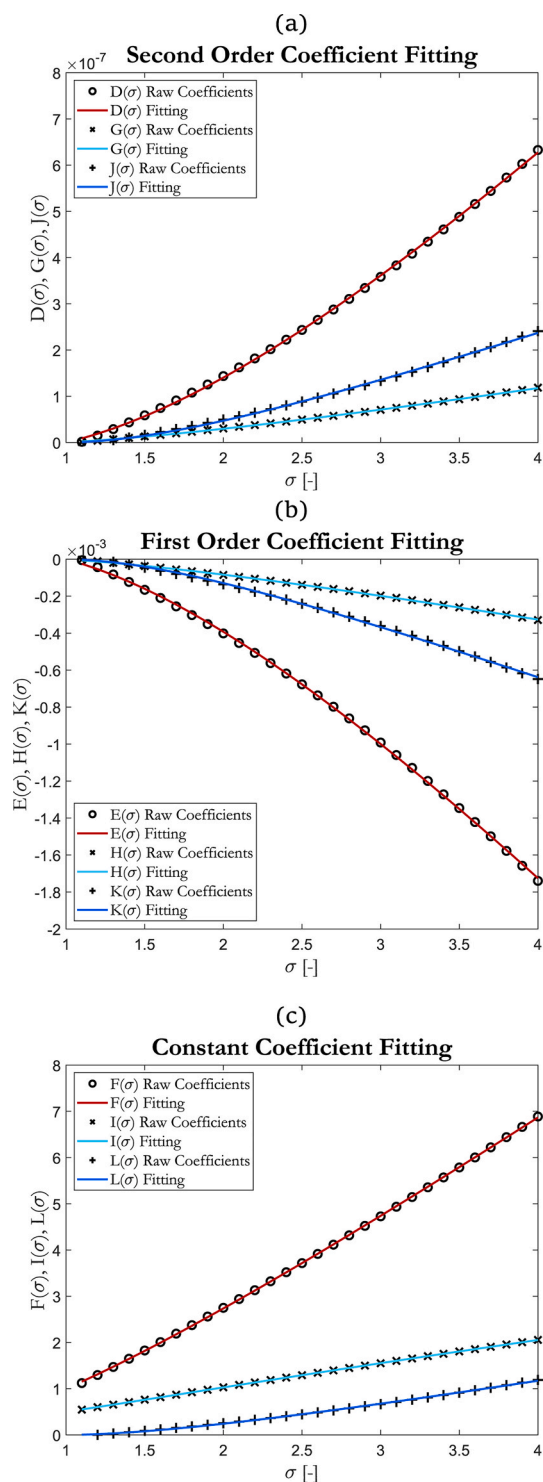


Fig. 3. Comparison between raw values and fitting functions of the second order (a), first order (b), and constant (c) coefficients of B_1 (red lines), B_2 (light blue lines), and B_3 (blue lines), with varying σ . (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

additional N_2 falls outside the neighbourhood of the reference state.

Given the comparable gradients obtained by considering either additional N_2 or substituting argon, it is possible to use the former approach to perform a chemical mechanism sensitivity on the computation of α . In fact, not all chemical schemes include argon. Fig. 6 shows α calculated with 10% of additional N_2 at 15 bar, with temperature set at

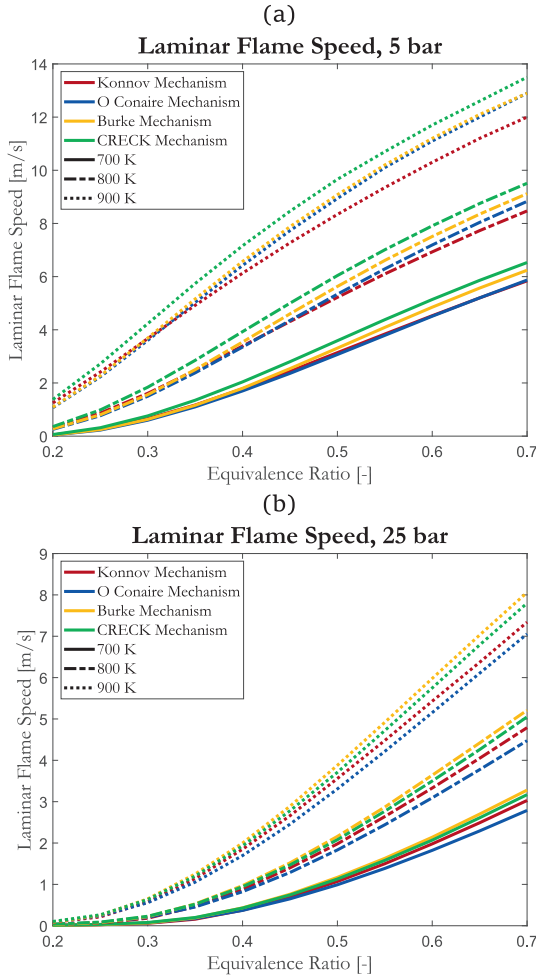


Fig. 4. Unstretched laminar flame speed computed at 5 bar (top) and 25 bar (bottom), at 700 K (solid lines), 800 K (dashed dotted lines), and 900 K (dotted lines), obtained with Konnov (red lines), O' Conaire (blue lines), Burke (yellow lines), and CRECK (green lines) mechanisms. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

700 K (a) and 900 K (b), and applying the same mechanisms previously seen in the laminar flame speed sensitivity analysis. As expected, comparable results are obtained in a wide range of equivalence ratios, at both temperatures. Differences arise with ultra-lean mixtures, particularly with equivalence ratios lower than the one corresponding to the local minimum of α . At these conditions, the Burke mechanism leads to slightly lower α , leading to higher ω_2 values. However, given the similar results obtained with mixtures richer than the one corresponding to the local minimum, and to be consistent with [17], the Burke mechanism will be considered in the following analyses.

The computation of α is performed by considering five different cases (detailed in Table 1), as two levels of argon substitution and three levels of N_2 addition are set. A fitting procedure of α is performed, and a different ω_2 map is obtained for each case.

The thermodynamic conditions for the fitting procedure are $0.2 \leq \Phi \leq 0.7$, $10 \text{ bar} \leq p \leq 50 \text{ bar}$, and 700 K . A two-term gaussian function α_{fit} , shown in Eq. (32), is found to well reproduce the chemical kinetics simulation data in the whole range considered, with $M(p)$, $N(p)$, $O(p)$, $P(p)$, $Q(p)$, and $R(p)$ calculated as in Eq. (33)-Eq. (38). As similar trends of α are found with all the cases considered, it is possible to fit the data using the same function type, modifying only the coefficients c_i , which are reported in Appendix A. As for Φ_{mod} , it is a function built to include the effect of the unburnt temperature, and it will be further discussed

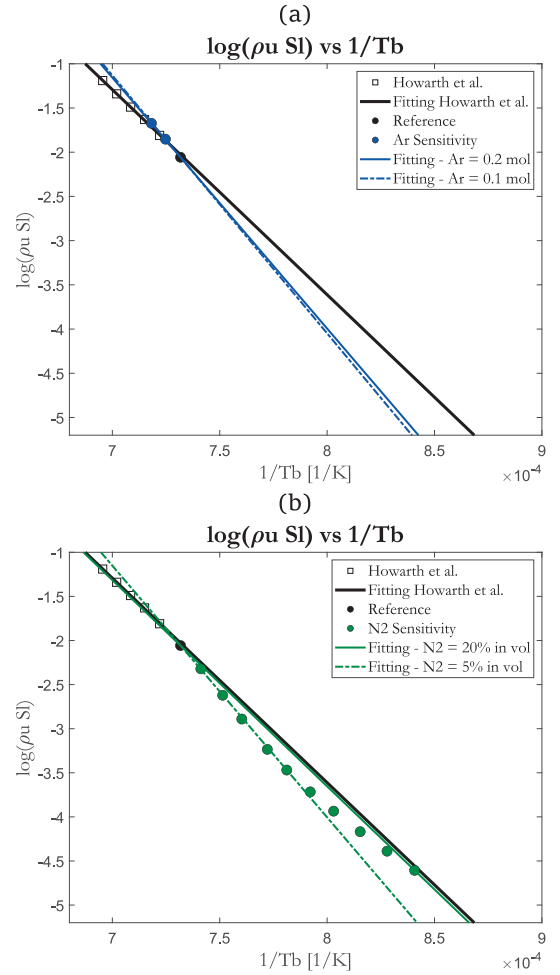


Fig. 5. Comparison of $\log(\rho_u S_L)$ against $1/T_b$ between literature data [17] and the results obtained in this work with argon substitution (a) and additional N_2 (b) approaches.

afterwards.

$$\alpha_{\text{fit}}(p, T, \Phi) = M(p) \bullet \exp \left(- \left(\frac{\Phi_{\text{mod}}(\Phi, T) - N(p)}{O(p)} \right)^2 \right) + P(p) \bullet \exp \left(- \left(\frac{\Phi_{\text{mod}}(\Phi, T) - Q(p)}{R(p)} \right)^2 \right) \quad (32)$$

$$M(p) = c_1 \bullet p^{c_2} \quad (33)$$

$$N(p) = c_3 \bullet \log_{10}(p) + c_4 \quad (34)$$

$$O(p) = c_5 \bullet p + c_6 \quad (35)$$

$$P(p) = c_7 \bullet p + c_8 \quad (36)$$

$$Q(p) = c_9 \bullet \log_{10}(p) + c_{10} \quad (37)$$

$$R(p) = c_{11} \bullet p + c_{12} \quad (38)$$

3.3. Computation of ω_2 at 700 K

Once α is computed, β can be derived. An ω_2 map can be obtained after calculating Le_{eff} through Eq. (11). Fig. 7 shows the resulting maps obtained with 0.1 mol (a) and 0.2 mol (b) of substituting argon, and 1% (c), 5% (d) and 20% (e) of additional N_2 . A modified version of the map with 20% of N_2 is also presented (f), and it will be discussed in the

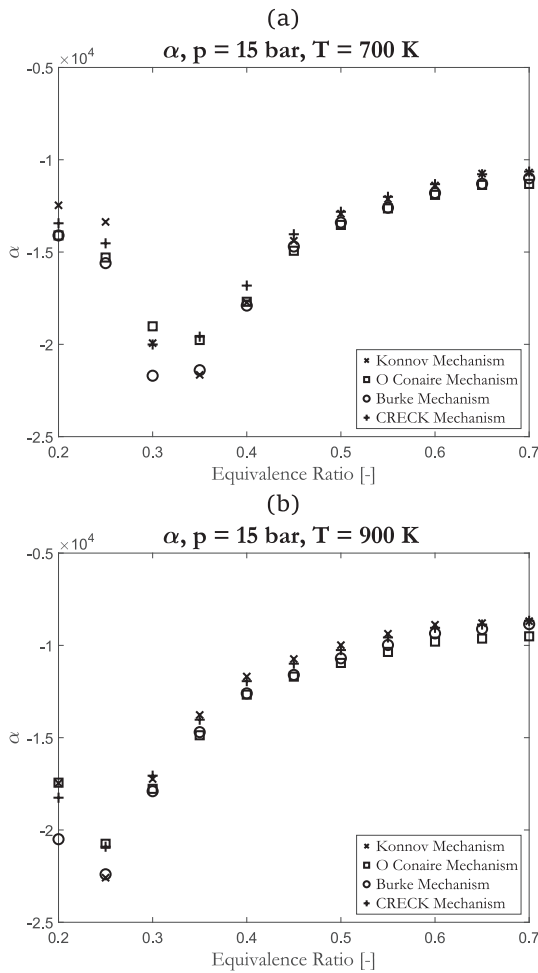


Fig. 6. α Calculated at 15 bar, 700 K (top) and 900 K (bottom), and $0.2 \leq \Phi \leq 0.7$, with Konnov (cross), O' Conaire (square), Burke (circle), and CRECK (plus) mechanisms.

Table 1

Cases considered for the computation of α .

Case A	Case B	Case C	Case D	Case E
Ar = 0.1 mol	Ar = 0.2 mol	N ₂ = 1% (in vol.)	N ₂ = 5% (in vol.)	N ₂ = 20% (in vol.)

following section. In these maps, the location of the theoretical most unstable surface (Eq. (13)) is provided (dashed line), together with the computed $\omega_2 = 0$ surface (solid line), for each case. As it can be seen, although the overall morphology of these maps are similar, resulting ω_2 values depend on the approach used to compute α , and a non-negligible difference can be noted for a given thermodynamic condition, as reported in Table 2.

As for the maps obtained with argon, results are comparable. For instance, the whole zone of high instability is characterized by similar ω_2 , as it is always within a 10% gap between the 0.1 mol (Case A) and 0.2 mol (Case B). Indeed, at 10 bar and with an equivalence ratio of 0.28, ω_2 is 11.47 and 11.03 for Case A and Case B, respectively.

With respect to the theoretical most unstable surface, although the trend is well captured, the computed surface is obtained with slightly richer mixture. The main discrepancies between the cases arise with mixtures with equivalence ratio higher than 0.4. Indeed, the ω_2 obtained with Case A is characterised by slightly higher values.

As for the N₂ sensitivity, the map obtained with 1% of N₂ (Case C) differs the most from the others. As it can be seen, there is a vast zone

where the instability parameter is negative, and the maximum values are lower than 5. As for the two cases with higher percentage of N₂, results are comparable and the overall morphology of these maps is similar to those in literature. For instance, the zone with higher ω_2 obtained with Case D and Case E is close to the theoretical most unstable surface. Although the computed equivalence ratios corresponding to the most unstable conditions are slightly overestimated, the trend is well captured in the whole thermodynamic range considered with both cases. Additionally, the trend of the $\omega_2 = 0$ threshold is in good agreement with the one presented in [17]. In terms of raw values, ω_2 is more than 30% higher in Case E, for Φ higher than 0.4, in the whole pressure range considered. In contrast, with Case D, the computed instability parameter is higher than Case F in the high-pressure zone.

3.4. Critical Φ modification

By considering either argon substitution or nitrogen addition, the computed most unstable surface is obtained with slightly richer mixture than the theoretical counterpart. In the high-instability zone, the highest ω_2 is obtained with Case A, while values closer to [17] are obtained with the additional N₂ approach (Case D and E). Fig. 8 depicts the ω_2 trend with Φ , at 700 K and 20 bar (a) or 40 bar (b), with Cases A, B, D and E.

In addition, the average ω_2 among the approaches is also reported (black dotted line), along with the theoretical Φ at which the highest ω_2 should be obtained following Eq. (13), renamed here Critical Φ . At both pressures, a steeper increase from $\Phi = 0.2$ up to the peak is noted with both argon amounts. As already mentioned, the Φ -wise location of the peak is slightly overestimated with respect to the theoretical one with all the tested approaches. However, the same overestimation is noted among the cases, with the exception of N₂ = 20% case where the critical equivalence ratio is 0.02 higher than the others. Considering the average profile, the computed critical Φ is 0.05 higher than the theoretical one at both pressures. After the maximum, which identifies the upper limit of the low-pressure zone, the rate of change of ω_2 is comparable with all approaches. At 20 bar, adopting Case A to compute ω_2 yields the strongest instability effect, with the unstretched laminar flame speed (Eq. (11) at $\Phi = 0.55$ increasing up to 30%, compared to 15% for Cases B and E, and 7% for Case D. At 40 bar and $\Phi = 0.55$, the lowest ω_2 is observed with Case D, with a flame speed increase of 18%, while the highest is obtained with Case A, with almost 37% of flame speed increase. These results suggest that the computed ω_2 is strongly dependent on the approach used to calculate β .

Given that the overestimation of the critical Φ is constant in the whole pressure range, an additional ω_2 map is generated to match the theoretical most unstable surface position. To do so, the function $N(p)$ (Eq. (34)), which represents the location of the first gaussian function peak, is modified. In particular, the value of c_4 is reduced by the average difference between the location of the theoretical peak and the computed one, for each case. The best agreement with literature in terms of ω_2 is obtained by modifying the case with 20% of N₂. Fig. 6f shows the resulting modified map. It can be noted that while the $\omega_2 = 0$ threshold does not vary with respect to the default setup, the computed and theoretical most unstable conditions are almost superimposed. The good agreement is also confirmed by the ω_2 values in Table 3. In fact, at 700 K, the most relevant difference can be noted at 20 bar and $\Phi = 0.2$, with the computed ω_2 equal to 3.69 against the literature value of 2.82.

3.5. Unburnt temperature dependency

As for the unburnt temperature dependency of α , results obtained with all the aforementioned approaches at every pressure considered show that the overall trend noted at 700 K with changing Φ can also be noted at different values of T_u . For instance, in Fig. 9, the scatter plots of α with 20% of additional N₂ at 20 bar and temperatures of 500 K, 700 K and 900 K are depicted. The black solid line represents the fitting function (Eq. (32)). By analysing the raw values from chemical kinetics

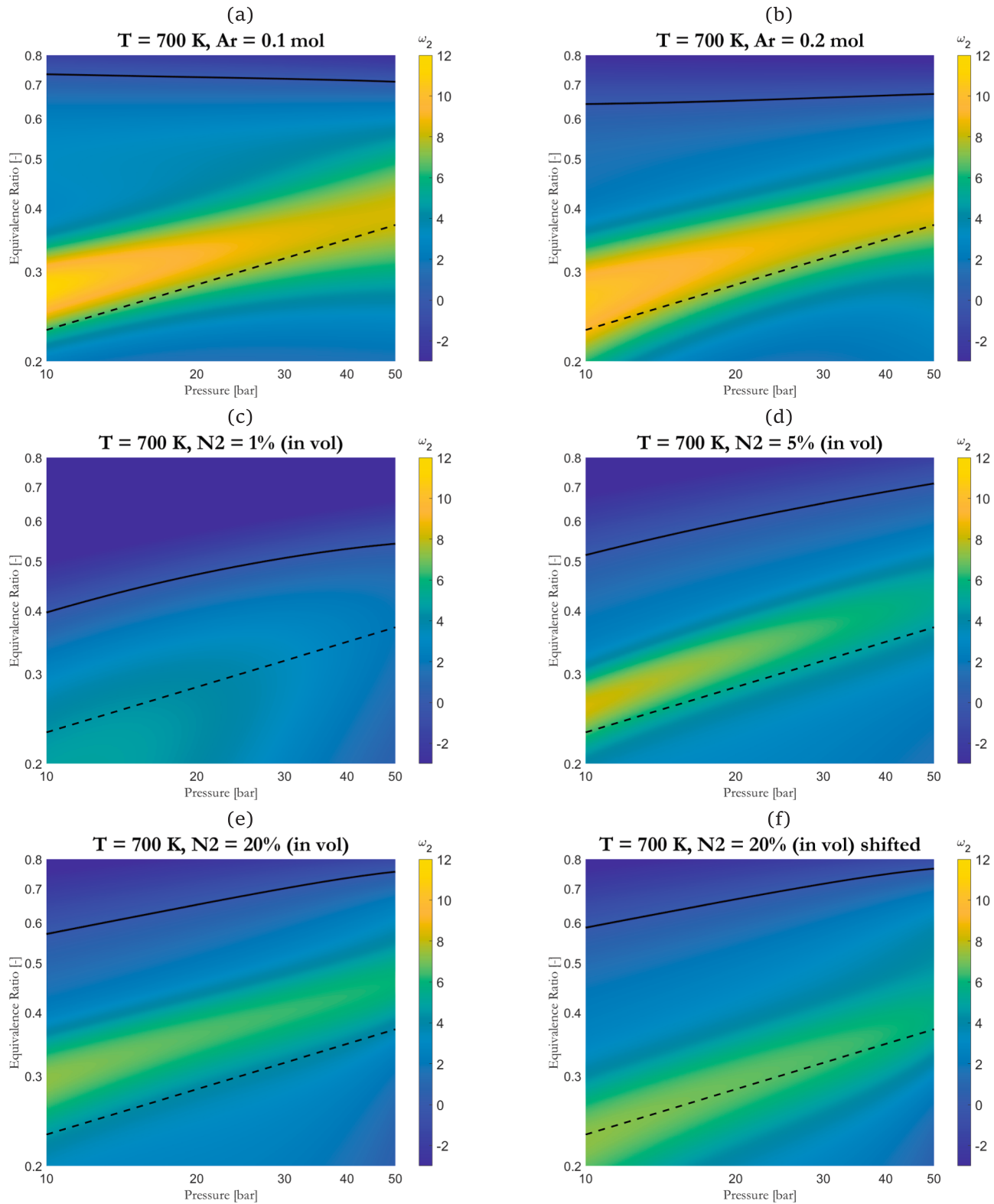


Fig. 7. Resulting ω_2 maps obtained with the proposed correlation, at 700 K, with 0.1 mol (a) and 0.2 mol of substituting argon (b), and 1% (c), 5% (d), and 20% of additional N_2 (e); (f) shows the application of the shifting function on (e) to match the theoretical most unstable surface. Theoretical most unstable surface (black dashed line) and calculated $\omega_2 = 0$ surface (black solid line) are also displayed.

simulations, it can be seen that the overall trend of α with Φ is nearly the same as that observed when varying the unburnt temperature. Indeed, the major difference that can be noted is the critical Φ , which is the value at which the local minimum occurs, which varies linearly with T_u . The

dotted lines are obtained by shifting the fitting function at 700 K towards leaner (red line) and richer mixtures (blue line) by the same amount as the difference in Φ_c among the cases. It is noteworthy that the function shifted towards richer mixtures well represents the results from

Table 2 ω_2 Comparison between literature data and resulting values obtained with the different approaches.

Temperature [K]	Φ [–]	Pressure [atm]	ω_2 [–]					
			Literature [17]	Ar = 0.1 mol (Case A)	Ar = 0.2 mol (Case B)	N ₂ = 1.0% in vol. (Case C)	N ₂ = 5.0% in vol. (Case D)	N ₂ = 20% in vol. (Case E)
700	0.2	20	2.82	1.49	1.96	4.13	2.89	2.71
	0.28	20	7.44	7.04	7.15	4.14	5.07	4.04
	0.4	10	2.71	3.00	2.45	–0.08	1.80	2.61
		20	4.22	5.32	5.34	2.03	3.73	5.66
		40	5.58	8.03	8.35	2.31	5.74	5.76

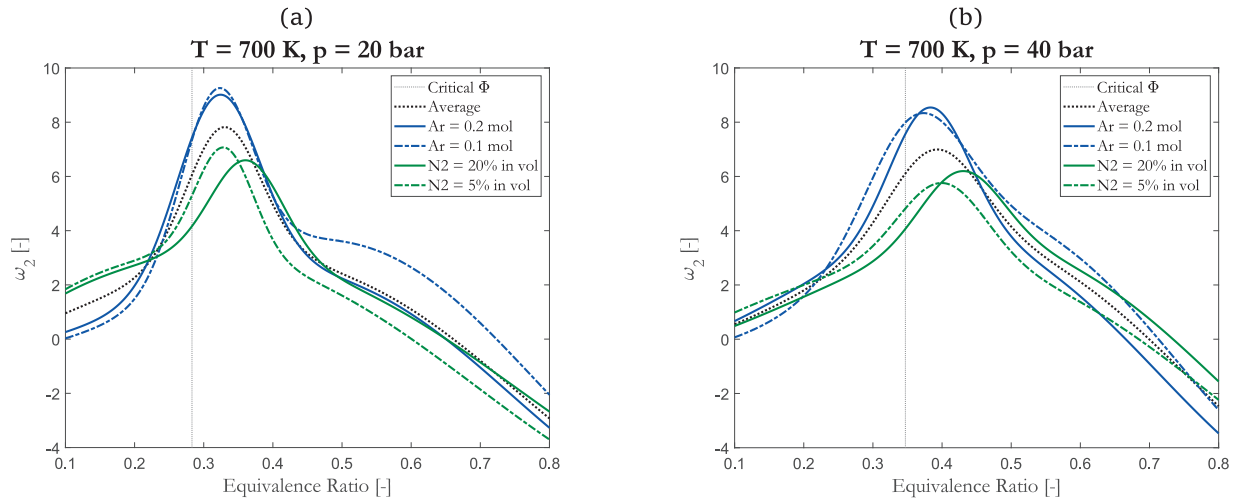


Fig. 8. Resulting ω_2 trends at 700 K and 20 bar (a) or 40 bar (b), with 0.1 mol (dashed-dotted blue lines) or 0.2 mol of substituting argon (solid blue lines), and 5% (dashed-dotted green line) or 20% of additional N₂ (solid green line). The average of these cases is also reported (dotted black line), along with the theoretical critical Φ . (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 3Comparison of ω_2 and I_0 between values obtained with the presented correlation and ones from literature. Blue values fall in the high pressure regime.

Temperature [K]	Φ [-]	Pressure [atm]	ω_2 [-]		ΔI_0 [%]
			Literature [17]	This Work (Case F)	
300	0.4	10	27.3	26.5	-2.7%
		20	17.1	15.3	-9.4%
		40	13.6	8.09	-35.0%
700	0.2	20	2.82	3.69	17.6%
	0.28	20	7.44	6.72	-5.6%
	0.4	10	2.71	2.40	-2.4%
		20	4.22	3.58	-5.0%
		40	5.58	5.72	1.1%

chemical kinetics at 500 K, with negligibly higher values for $\Phi < \Phi_c$. In contrast, at 900 K, the trend is very well captured by the fitting function shifted towards leaner mixtures, with only a slight overestimation of the local minimum, which leads to a slightly lower ω_2 . Therefore, by considering the linear dependence on the unburnt temperature, the $\Phi_{\text{mod}}(\Phi, T)$ function shown in Eq. (39) is considered when computing α through Eq. (32). It is worth noting that when T_u is 700 K, $\Phi_{\text{mod}} = \Phi$ and thus the starting α_{fit} is obtained.

$$\Phi_{\text{mod}}(\Phi, T) = \Phi + 0.0005 \cdot (T - 700) \quad (39)$$

As mentioned, the same dependency is found with all the approaches investigated in this work, and thus it can be applied to each proposed correlation. The resulting ω_2 maps, obtained with the shifted N₂ = 20% approach, at 500 K and 900 K can be seen in Fig. 10.

With temperatures up to 700 K, the high ω_2 zone is superimposed to

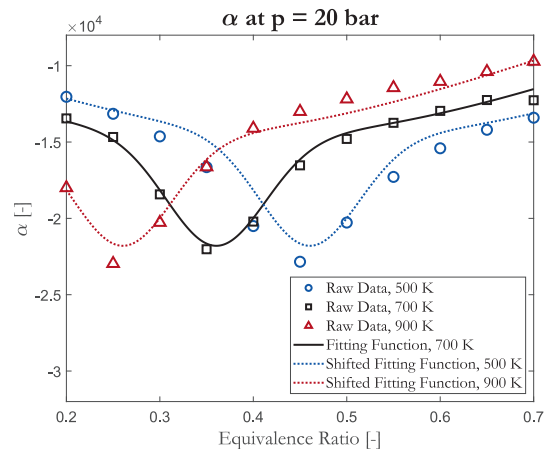


Fig. 9. Chemical kinetics data obtained at 20 bar (scatter plots) and temperatures of 500 K (blue), 700 K (black) and 900 K (red) are compared with the fitting function found in this work at 700 K (black solid line) and the shifted fitting functions towards richer (dotted blue line) and leaner (dotted red line) mixtures. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

the theoretical most unstable surface location in the whole pressure and equivalence ratio domains. In contrast, with temperatures higher than 700 K, a different dependency is necessary to match the theoretical value. In fact, at 900 K, the black dashed line falls outside the analysed $p - \Phi$ space, while the computed ω_2 map has the maximum values within the $0.2 \leq \Phi \leq 0.3$ and $20 \leq p \leq 50$ bar ranges. However, a two-step dependency is not considered here, as Eq. (39) is found to well

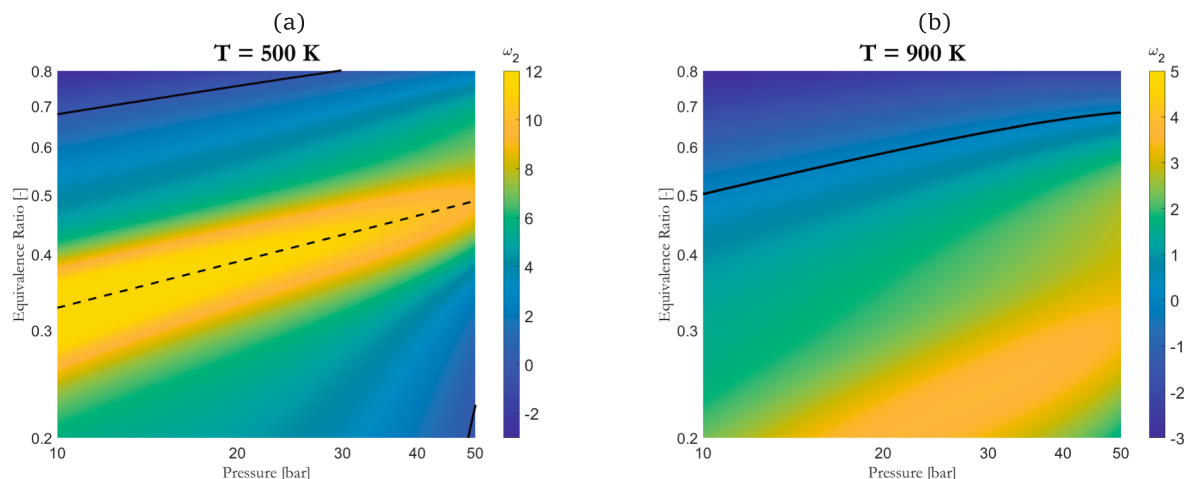


Fig. 10. Computed ω_2 map with the presented correlation at 500 K (a) and 900 K (b). The theoretical most unstable surface (black dashed line) and the calculated $\omega_2 = 0$ surface (black solid line) are also displayed.

reproduce the chemical kinetics results. Moreover, there is no evidence suggesting that the empirical correlation that defines the most unstable conditions (Eq. (13)) is accurate with such temperatures.

As a further assessment of this methodology, Table 3 reports the comparison at 300 K between [17] and this work. The latter values are obtained by extrapolation from the developed function. A good agreement can be found, with the sole exception of the 40 bar and $\Phi = 0.4$ point. However, it is important to note that this condition is not relevant in the ICE case, given its high pressure and low temperature. Considering all the data reported in Table 3, the main differences in terms of flame speed increase can be found in the high-pressure zone, reported in blue. For instance, an overestimation of 17.6% of the flame speed increase is found at 20 atm, 700 K and with an equivalence ratio of 0.2. However, a good agreement is noted in the low-pressure zone, as the highest difference can be found at $\Phi = 0.28$, 700 K and 20 atm, with an underestimation of 5.6%.

Finally, Fig. 11 depicts the ω_2 trends at 500 K and 700 K, both at 20 bar, obtained with $N_2 = 20\%$ and the shifted correlation, to show the effect of both Φ_{mod} and the change of c_4 in Eq. (34). As shown, modifying c_4 causes a shift in the Φ -wise location only of the peak of ω_2 , to match the theoretical critical Φ , while the former covers well the instability increase due to temperature decrease.

3.6. Extrapolation at engine-like conditions

As stated in the previous sections, the proposed correlation is developed through a fitting procedure of chemical kinetics simulations performed from 10 bar to 50 bar. Although results are in good agreement with literature data, the applicability of such method may be limited. For instance, in hydrogen-fuelled engines, only the light-duty architectures with low power output operating conditions can be tested, as the maximum pressure and temperature may fall outside of the prescribed validity range of the method proposed. However, one of the key advantages of using a correlation-based approach is the possibility to extrapolate data. Indeed, in the previous section, a good agreement with literature data in terms of raw ω_2 values at 300 K is noted, even though the lowest temperature value considered for the development of the α_{fit} function is 500 K. Therefore, to assess the robustness of the proposed approach, the performance of the Case A correlation is analysed at higher pressure and temperature conditions.

Fig. 12 shows the correlation obtained with 0.1 mol of substituting argon at 900 K (a) and 1100 K (b). Additionally, the pressure ranges from 10 bar to 100 bar. Firstly, it is noteworthy that the temperature dependence is once again well captured, as the overall morphology of the map is maintained, while the ω_2 values decrease with increasing

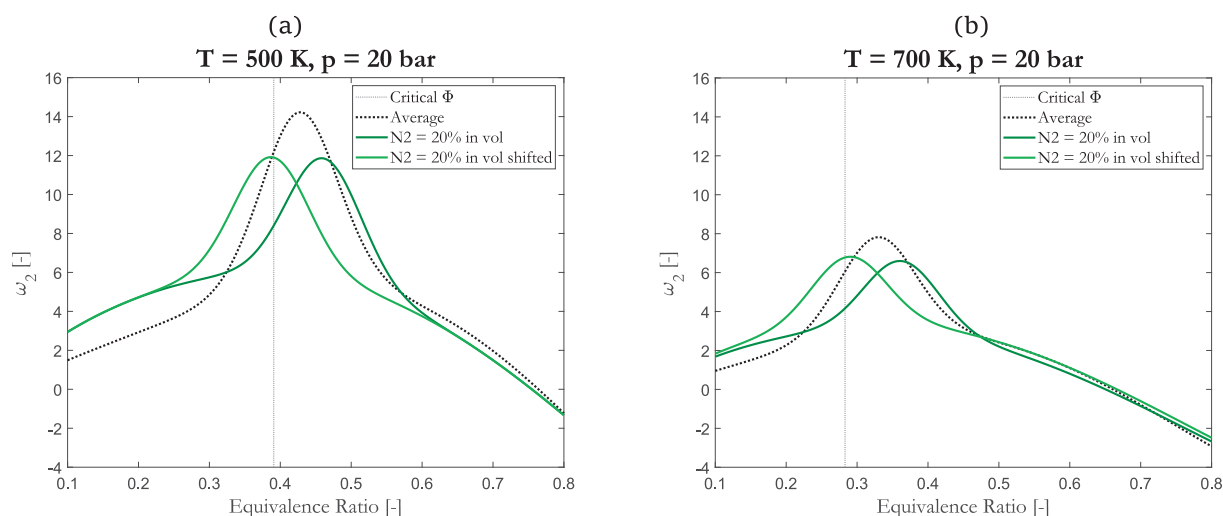


Fig. 11. Resulting ω_2 trends at 500 K (a) and 700 K (b), obtained with 20% of additional N_2 , with (light green line) and without (green line) the modification to match the critical Φ (dotted grey line). The average of all the cases without modification is also reported (dotted black line). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

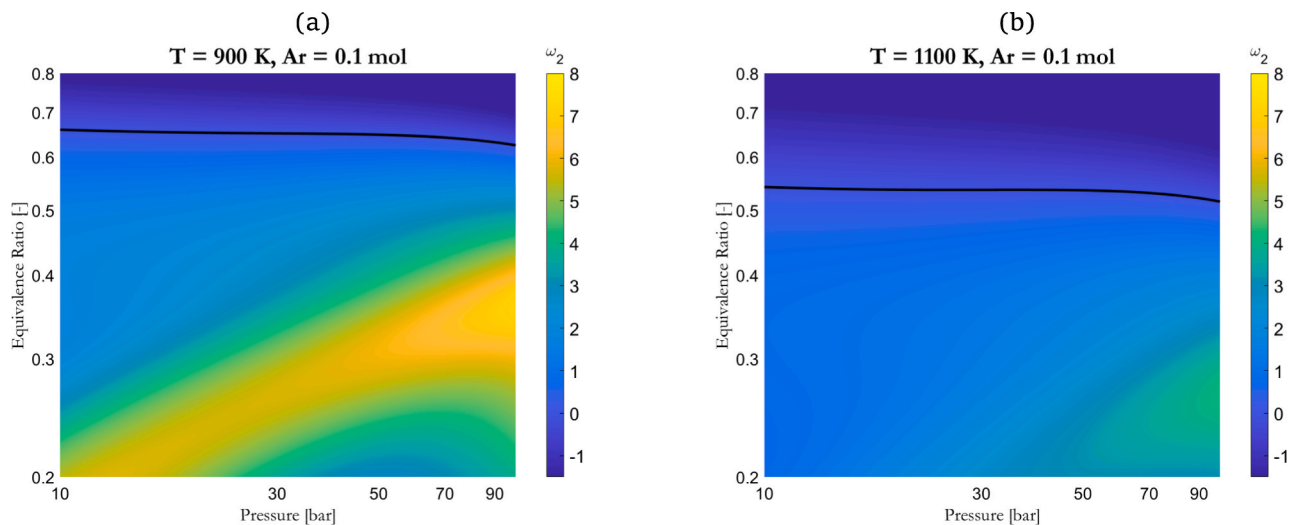


Fig. 12. Computed ω_2 map with the presented correlation at 900 K (a) and 1100 K (b) up to 100 bar. The calculated $\omega_2 = 0$ surface (black solid line) is also displayed.

temperature. With a given temperature, the $\omega_2 = 0$ threshold remains almost constant throughout the pressure range: at 900 K, the threshold can be found between $\Phi = 0.6/0.7$, while at 1100 K between $\Phi = 0.5/0.6$. The performance of the correlation gets slightly worse with pressure values higher than 90 bar. For instance, in the neighbourhood of the most unstable surface at 900 K (Fig. 12a), it is possible to note that above 90 bar, the second order instability parameter start to increase. This is related to the mathematical definition of the α_{fit} function, and particularly to the interaction between the two gaussian function adopted. However, with increasing temperature this bulge shifts towards even higher pressures, which broadens the applicability of such correlation.

4. Conclusions

As shown in several works in literature, ω_2 can be effectively used to include the effect of thermo-diffusive instabilities on the unstretched laminar flame speed propagation of hydrogen-air flames through an empirical model. The computation of this parameter involves several non-trivial steps, such as the calculation of B_i values and the Zel'dovich number β . Particularly, the last step requires one-dimensional chemical kinetics simulations, which makes the implementation of this methodology difficult in a CFD framework. In this work, a correlation to compute the second order instability parameter ω_2 in a range of engine-like thermodynamic conditions is proposed. Firstly, the thermal expansion parameter is computed with one-dimensional chemical kinetics in a wide range of thermodynamic conditions. Secondly, the computation of B_i is considered, and a fitting procedure deployed. Thirdly, the calculation of β is analysed and a chemical mechanism sensitivity is performed. Moreover, different approaches concerning the computation of the activation energy of the mixtures, such as the substitution of a small amount of N_2 with the same amount of argon and the addition of N_2 , are examined, and a fitting procedure deployed. It is possible to conclude that:

- σ can be described through a second order polynomial function in Φ and T_u , while the pressure dependence within the analysed range can be neglected.
- By calculating the thermal conductivity of the mixture $\lambda(x)$ through the Sutherland's law, B_1 , B_2 , and B_3 can be described with a second order polynomial function in Φ and T_u .
- A two-term gaussian function in Φ and p is found to well fit the activation energy trend found through chemical kinetics simulations at 700 K. Concerning the temperature dependence, an almost rigid

shift of α is noted with varying T_u , and a linear dependency of T_u is included in the effective equivalence ratio entering the fitting function of α .

- Although the overall ω_2 maps are comparable to the ones that can be found in the literature, both the adopted approaches to compute the activation energy and the chosen amount of substituting argon or additional N_2 have a non-negligible impact on the raw ω_2 values. For instance, with a $\Phi = 0.55$ mixture at 20 bar and 700 K, the laminar flame speed increase is 7% if calculated with 5% of additional N_2 , 15% when using 0.2 mol of substituting argon or 20% of additional N_2 , and 30% with 0.1 mol of argon.
- As for the activation energy of the mixture, comparable results are obtained with different chemical mechanisms in the whole range of considered pressure, temperature and equivalence ratio. Hence, the overall conclusions drawn from this work are independent from the chemical mechanism used.
- By applying the proposed correlations, the one with 0.1 mol of substituting argon (case A) is expected to give the highest flame speed enhancement in a broad range of thermodynamic conditions, while the lowest effect on the flame development is expected if the correlation obtained with 5% of additional N_2 (case D) is adopted.
- The better agreement with literature data, which were obtained with the argon substitution method, is found with the correlation obtained with 20% of additional N_2 . Additionally, to match the most unstable surface location, a calibration of the gaussian term was required (Case F).
- One of the key advantages of the proposed approach is the extrapolation capability. For instance, although the correlation was developed through chemical kinetics simulations up to 50 bar and between 500 K and 900 K, a good agreement with literature data at 300 K can be found. Furthermore, by extrapolating the Case A correlation, reasonable ω_2 trends are observed up to 100 bar and 1100 K.

The proposed correlation fills a gap found in literature, as it allows the readers to include the effect of hydrogen thermo-diffusive instability in their numerical setup regardless of the CFD code and combustion model deployed, as only the pressure, temperature and equivalence ratio of the mixture are needed. Further studies will include the effect of exhaust gas recirculation on the ω_2 calculation, along with the extension of the thermodynamic range of validity of the correlation. Indeed, reasonable ω_2 trends can be found with higher pressure and temperature values through extrapolation. Nevertheless, validation against chemical kinetics data could be necessary, allowing a re-calibration of the c_i parameters to extend the validity of the proposed approach. Finally, in-

cylinder simulations will be adopted to assess the effect on flame propagation of the application of the different developed fitting functions.

CRediT authorship contribution statement

Manuel Madia: Writing – original draft, Visualization, Validation, Methodology, Formal analysis, Data curation, Conceptualization. **Fabio Berni:** Writing – review & editing, Writing – original draft, Validation, Supervision, Formal analysis, Data curation, Conceptualization. **Alessandro d’Adamo:** Writing – review & editing, Validation, Supervision, Formal analysis, Data curation, Conceptualization. **Stefano Fontanesi:** Writing – review & editing, Supervision, Resources, Methodology, Formal analysis, Conceptualization. **Sebastiano Breda:** Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Methodology, Formal analysis, Data curation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A.: Coefficients of the correlation

Table 4
Coefficients for Eqs. (15)–(17).

a_1	−1.309E-06
a_2	4.076E-03
a_3	−3.885E + 00
a_4	3.637E-06
a_5	−1.077E-02
a_6	9.627E + 00
a_7	1.058E + 00

Table 5
Coefficients for Eqs. (22)–(30).

b_1	2.989E-08
b_2	6.527E-08
b_3	−1.064E-07
b_4	−7.904E-05
b_5	−1.950E-04
b_6	3.047E-04
b_7	9.000E-02
b_8	1.529E + 00
b_9	−6.698E-01
b_{10}	3.910E-09
b_{11}	2.070E-08
b_{12}	−2.670E-08
b_{13}	−1.030E-05
b_{14}	−6.010E-05
b_{15}	7.610E-05
b_{16}	−8.137E-03
b_{17}	5.619E-01
b_{18}	−6.240E-02
b_{19}	1.190E-08
b_{20}	2.430E-08
b_{21}	−4.660E-08
b_{22}	−3.070E-05
b_{23}	−7.200E-05
b_{24}	1.310E-04
b_{25}	5.548E-02
b_{26}	1.354E-01
b_{27}	−2.404E-01

Table 6
Coefficients for Eqs. (32)–(38).

	Ar = 0.1 mol (Case A)	Ar = 0.2 mol (Case B)	N ₂ = 1.0% in vol. (Case E)	N ₂ = 5.0% in vol. (Case D)	N ₂ = 20% in vol. (Case C)	N ₂ = 20% in vol. shifted (Case F)
c ₁	−8.908E + 04	−8.486E + 04	−4.641E + 04	−4.195E + 04	−2.707E + 04	−2.707E + 04
c ₂	−6.199E-01	−5.979E-01	−3.291E-01	−5.447E-01	−4.462E-01	−4.462E-01
c ₃	1.366E-01	2.043E-01	4.905E-01	2.318E-01	2.192E-01	2.192E-01
c ₄	1.379E-01	5.143E-02	−4.207E-01	2.601E-02	7.469E-02	0.000E + 00
c ₅	1.342E-03	−1.969E-04	−7.518E-04	1.424E-03	4.346E-04	4.346E-04
c ₆	4.614E-02	8.807E-02	3.558E-01	3.107E-02	6.515E-02	6.515E-02
c ₇	−6.075E + 01	−1.131E + 02	0.000E + 00	−1.390E + 01	−9.409E + 01	−9.409E + 01
c ₈	−1.579E + 04	−1.213E + 04	0.000E + 00	−1.432E + 04	−1.282E + 04	−1.282E + 04
c ₉	−8.035E-02	−1.110E-01	0.000E + 00	4.964E-01	4.541E-01	4.541E-01
c ₁₀	6.257E-01	6.219E-01	0.000E + 00	−3.257E-01	−2.090E-01	−2.090E-01
c ₁₁	−1.634E-03	−1.256E-03	0.000E + 00	−1.620E-03	−8.073E-03	−8.073E-03
c ₁₂	4.503E-01	4.686E-01	0.000E + 00	6.260E-01	8.073E-01	8.073E-01

Data availability

No data was used for the research described in the article.

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