

# Experimental and numerical determination of Lewis number and Markstein lengths for a multi-component jet fuel surrogate and air mixtures

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## 1 Introduction

This study focuses on the thermodiffusive instabilities formation of spherical premixed flames. The conditions under which these instabilities develop must be characterized for a better understanding and a better control of this regime. The instabilities are described by the emergence of wrinkling and cells overall the flame front surface. Thus, when instabilities occur, the flame front surface becomes larger, increasing the consumption rate of fresh gases. The flame front is more and more unstable, new cells are generated and the flame front speed is faster: instabilities are self-sustained and the flame front is self-accelerated. When combustion takes place in constant volume chamber, the combustion process induces a pressure increase that favours the instabilities.

The thermodiffusive instabilities are generated when the molecular diffusivity is larger than the thermal diffusivity. That corresponds to a low value of Lewis number, defined by the ratio of thermal diffusivity  $\alpha$  of the mixture to the molecular diffusivity  $D_{i,j}$  of the limiting reactant:

$$Le = \frac{\alpha}{D_{i,j}} \quad (1)$$

where the thermal diffusivity is expressed from the thermal conductivity  $\lambda_u$ , the density  $\rho_u$  and the heat capacity at constant pressure  $C_{p,u}$  by the equation  $\alpha = \lambda_u \rho_u^{-1} C_{p,u}^{-1}$ .

A mixture with a Lewis number lower than the critical Lewis number (slightly lower than unity) is unstable in the thermodiffusive sense, and on the contrary, a mixture with a Lewis number higher than a critical Lewis number is considered as stable. Estimation of the Lewis number of mixtures is the parameter to control flame front thermodiffusive stability. The determination of Lewis number for a mixture with a mono-component

## **Le Dortz, R. Determination of Lewis number and Markstein lengths for jet fuel surrogate and air mixtures**

fuel is obvious, but becomes hardest for multi-component fuels, because all species have to be taken into consideration in the overall mixture. To the knowledge of the authors, only two recent studies have dealt with the elaboration of a methodology to evaluate the Lewis number for mixtures with a multi-component fuel, and especially for syngas [1-2]. Although some *n*-alkanes were employed in the previous mentioned studies, evaluation of Lewis number for mixtures only constituted with hydrocarbons have not been realized yet.

The objective of this study is to formulate a numerical methodology to predict the conditions promoting the formation of such thermo-diffusive instabilities for a multi-component jet fuel surrogate: the Dagaut surrogate constituted with 74 % *n*-decane, 15 % *n*-propylcyclohexane and 11 % *n*-propylcyclohexane [3]. This methodology is also evaluated comparing the results with spherical flame experimental data through the measurements of Markstein lengths (ML). Indeed, the ML is directly in relation with the Lewis number (see Eq. (3)). A negative ML corresponds to a Lewis number lower than the critical value, and vice versa.

## **2 Methodology**

### **2.1 Experimental set-up**

The spherical combustion chamber employed in this study was already presented during the 26<sup>th</sup> ICDERS meeting [4]. The vessel is a stainless-steel spherical chamber with a 4.2 L inner volume (0.2 m in diameter) and equipped with two UV-sapphire optical access windows (0.07 m in diameter) to ensure optical measurements. This experimental set-up was designed to support initial pressures up to 1.0 MPa and initial temperatures up to 470 K. Ignition of the mixture is initiated by an electrical discharge (inductive circuit with plug top coils) of around 20 mJ between two pin-to-pin tungstene electrodes with a 1 mm gap. Pressure during combustion is measured using a piezoelectric dynamic pressure transducer Kistler 6054 AR 0-250 bar coupled with a Kistler ICAM amplifier Type 5073A. The propagation of the flame is recorded using a Schlieren visualization system constituted with a high speed camera Photron FASTCAM SA5 at a frame recording rate of 7 kHz and a collimated LED Opto Engineering as a light source. Frame resolution is 1,024\*1,024 pixels<sup>2</sup> with an exposure time fixed to 4.5  $\mu$ s. Measurements (pressure and visualization) are synchronized with the onset of the ignition. The ML are determined simultaneously with the unstretched laminar burning velocity using the non-linear extrapolation of Kelley and Law [5] as presented in [4].

### **2.2 Lewis number and Markstein lengths numerical determination**

The determination of the effective Lewis number of a premixed flame constituted with air and a multi-component jet fuel is realized in 3 different steps detailed in Bouvet et al. [1] and Lapalme et al. [2]:

1. Evaluation of Lewis number  $Le_i$  for each specie of the multi-component fuel with 3 different methods.
2. Evaluating the Lewis number of the multi-component fuel  $Le_{fuel}$  using Lewis numbers  $Le_i$  from each specie: three formulations are proposed in literature to calculate the multi-component fuel Lewis number by weighting the different  $Le_i$  (volume-based (V), diffusion-based (D) and heat-release based (H) formulations).

**Le Dortz, R. Determination of Lewis number and Markstein lengths for jet fuel surrogate and air mixtures**

3. Association of the Lewis numbers of the fuel  $Le_{fuel}$  and the oxidizer  $Le_{Ox}$  for evaluating the effective Lewis number  $Le_{eff}$  of the mixture following the classical approach proposed by Bechtold and Matalon [6] for a mixture constituted with a fuel and an oxidizer.

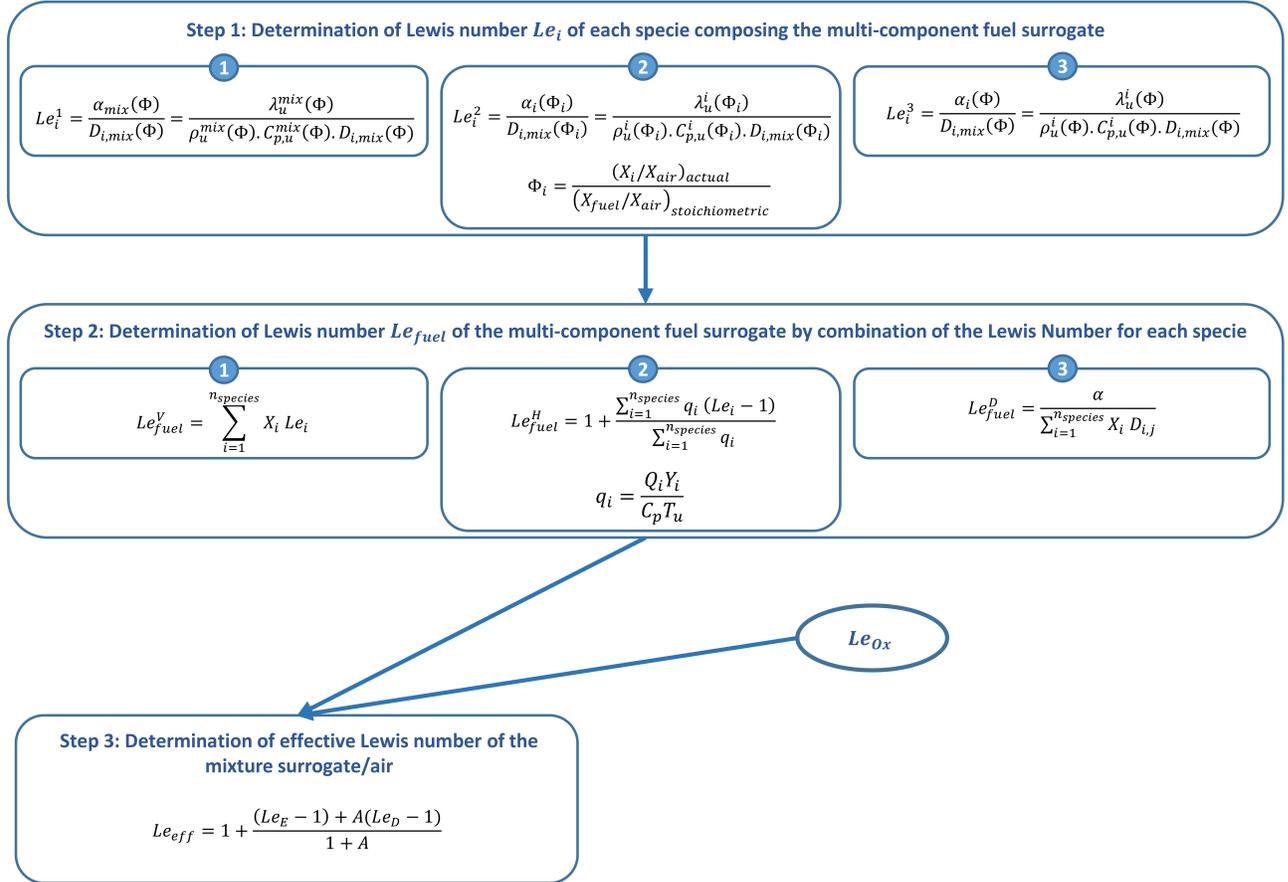


Figure 1: Methodology for determination of Lewis number for multi-component surrogate and air mixtures - Notations for Fig. 1:  $\alpha$ : thermal diffusivity ;  $D$ : molecular diffusivity ;  $\lambda$ : thermal conductivity ;  $\rho$ : density ;  $C_p$ : specific heat at constant pressure ;  $X$ : molar fraction ;  $q_i$ : non-dimensional heat release defined by  $q_i = Q_i Y_i C_p^{-1} T_u^{-1}$  with  $Q$ : heat of reaction,  $Y_i$ : mass fraction,  $T_u$ : fresh gases temperature ;  $Le_E$ : Lewis number of excessive reactant ;  $Le_D$ : Lewis number of deficient reactant ;  $A = 1 + Ze(\theta - 1)$  with  $Ze$ : Zel'dovich number defined after and  $\theta$  defined as  $\theta = 1/\Phi$  for  $\Phi \leq 1$  and  $\theta = \Phi$  for  $\Phi > 1$ . Also, subscripts or superscripts  $i$  and  $mix$  identifies the property applied respectively to the specie  $i$  and the mixture  $mix$

The methodology is synthesized in Fig. 1 and conducts to 9 different evaluations of effective Lewis Number. Also, when mixtures are very rich (equivalence ratio  $\Phi > 1.2$ ) and very low ( $\Phi < 0.8$ ), the use of Bechtold and Matalon's formulations to estimate the effective Lewis number don't provide a good reproducibility of experimental results [1,2]. The weighting does not allow a transition to an unstable flame regime: Lewis number is always higher than the critical Lewis number. That's why the formulation of Bechtold and Matalon must be employed only for near stoichiometric mixtures ( $0.8 < \Phi < 1.2$ ). Outside this range of equivalence ratios, the effective Lewis number is equal to the Lewis number of the limiting

specie ( $Le_{eff} = Le_{fuel}$  for  $\Phi < 0.8$  and  $Le_{eff} = Le_{Ox}$  for  $\Phi > 1.2$ ).

However, this modification is quite abrupt and implies a discontinuity at the pivotal equivalence ratios. In order to obtain a more continuous and smooth evolution of the effective Lewis number, a progressive transition is used:

$$Le_{eff} = \begin{cases} Le_{fuel} & \text{if } \Phi \leq 0.6, \\ 2.5(1 - \Phi) Le_{fuel} + (2.5\Phi - 1.5) Le_{BM} & \text{if } 0.6 \leq \Phi \leq 1, \\ 2.5(\Phi - 1) Le_{Ox} + (-2.5\Phi + 3.5) Le_{BM} & \text{if } 1 \leq \Phi \leq 1.2, \\ Le_{Ox} & \text{if } \Phi \geq 1.2. \end{cases} \quad (2)$$

where  $Le_{BM}$  is the Lewis number defined by Bechtold and Matalon.

Finally, the ML is expressed from Lewis number with the relation which best corresponds for hydrocarbons/air premixed flames (Eq. (3)). Indeed, other relation exist [6-7] but are more adapted for premixed flames with hydrogen basis. The burnt Markstein length  $\mathcal{L}_b$  is expressed with the following relation of Chen [8]:

$$\mathcal{L}_b = \left[ \frac{1}{Le} - \left( \frac{Ze}{2} \right) \left( \frac{1}{Le} - 1 \right) \right] \sigma \delta_f \quad (3)$$

where  $Ze$  is the Zel'dovich number,  $\sigma$  is the expansion factor defined by the ratio of fresh gases density with burnt gases density  $\rho_u/\rho_b$  and  $\delta_f$  represents the flame front thickness. The Zel'dovich number is a non-dimensional parameter which corresponds to the reactivity of the mixture and defined by the relation  $Ze = Ea(T_{ad} - T_u)/(RT_{ad}^2)$ , with  $Ea$  the activation energy,  $T_{ad}$  and  $T_u$  are respectively the burnt gases and fresh gases temperatures. All these previous parameters are calculated using Cantera chemical code [9] and the transport properties associated to the Luche reduced chemical mechanism [10].

### 3 Results

#### 3.1 Influence of the Lewis number calculation methodology on Lewis number and Markstein length evaluations

Fig. 2.a represents the Lewis number plotted against equivalence ratio for a premixed flame of Dagaut surrogate and air at initial temperature  $T_0 = 400$  K and initial pressure  $P_0 = 0.1$  MPa. Very few differences appear between the different methodologies: main differences between the Lewis number occur for lean mixtures, with a variation of Lewis number equal to 0.25 between methods at  $\Phi = 0.6$ . For rich mixtures, the Lewis numbers are the same for all methodologies because the Lewis number corresponds to the Lewis number of the limiting specie.

The ML as a function of equivalence ratio is represented on Fig. 2.b. In terms of notations, as an example, the effective Lewis number of mixture noted  $Le^{V1}$  has been calculated using the expression of  $Le_{fuel}^V$  for associating the Lewis numbers of each specie, estimated using the definition  $Le_i^1$ . As pointed out by Lapalme et al. [2], the choice of the definition for the Lewis number of each fuel specie do not have any influence on the results.

More surprisingly, the choice of methodology for associating the Lewis number of each specie do not also have any influence for the estimation of the Lewis number. Bouvet et al. and Lapalme et al. have underlined in their respective study an influence of the model chosen for associating Lewis number of each specie in the case of hydrogen, syngas and hydrocarbons premixed flames. By analysing more deeply the results of Bouvet et al. [1] and Lapalme et al. [2], and coupling their results with those of this study, it seems that the association model does not have any influence on the results when the species are from the same nature (here hydrocarbons), because the Lewis numbers of the species are very close one from another.

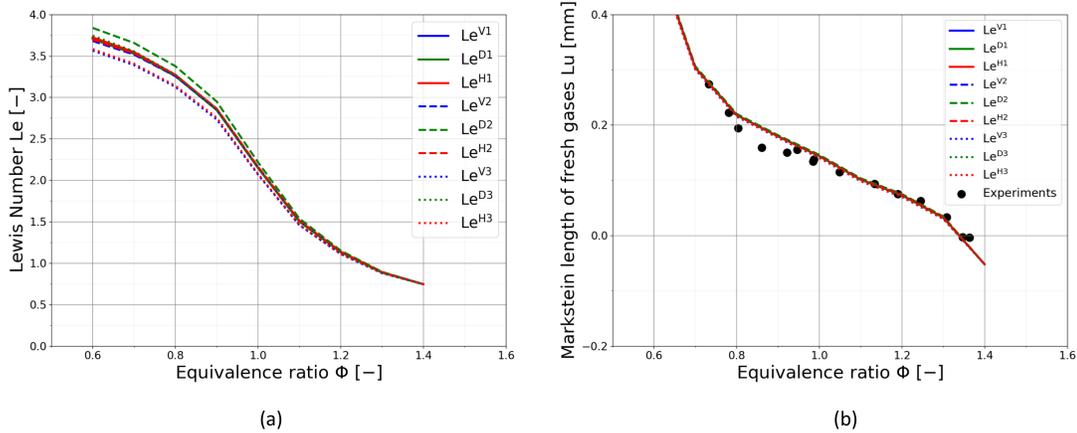


Figure 2: (a) Lewis Number and (b) Experimental and numerical Markstein lengths versus equivalence ratio for a premixed flame of Dagaut surrogate and air at initial temperature  $T_0 = 400$  K and  $P_0 = 0.1$  MPa - Comparison between the different Lewis number calculation methodologies

### 3.2 Thermo-diffusive instabilities formation

Comparison of experimental and numerical ML for Dagaut surrogate and air premixed flames at different initial conditions is presented in Fig. 3. Experimental results are taken from the study of Le Dortz et al. [4] presented during the 26<sup>th</sup> ICDERS meeting. Numerical results confirm the analysis in ref. [4] concerning the temperature effects on the front flame thermodiffusive stability, i.e. there is no influence of initial temperature on the stability of the mixture. However, numerical simulations do not confirm the influence on initial pressure on the front flame stability, experimentally observed by measurements of ML: experimental measurements highlight a transition to an unstable flame with an equivalence ratio  $\Phi = 1.2$  when initial pressure is  $P_0 = 0.3$  MPa, whereas this transition happens with  $\Phi \approx 1.35$  when  $P_0 = 0.1$  MPa. For numerical cases, the transition from stable to unstable front flame is the same for all tested conditions and occurs for  $\Phi = 1.33$ , implying that the thermodiffusive instability depends only on the nature of the mixture, and not initial conditions (pressure and temperature). On the contrary, experimental measurements indicates a link between thermodiffusive instabilities formation and increases of pressure and equivalence ratio. Nevertheless, numerical simulations are able to reproduce correctly the behavior of experimental ML overall tested conditions.

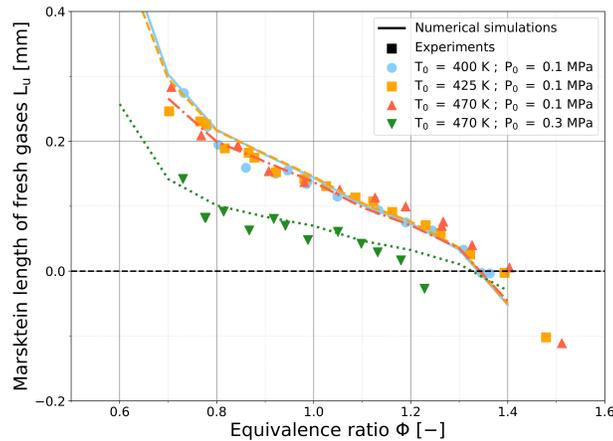


Figure 3: Experimental and numerical Markstein lengths versus equivalence ratio for a premixed flame of Dagaut surrogate and air at different initial temperatures and pressures

## 4 Conclusion

A methodology dedicated to evaluate the Lewis number of a premixed flame realized with a multi-component fuel has been proposed in this study to establish the formation of thermodiffusive instabilities on the flame front: the different species of the fuel are associated according to the volume fraction of each specie, and then coupled with air according to the classical formulation of Betchold and Matalon. This methodology is able to reproduce with a good correlation the results obtained using experimental techniques excepted for the pressure influence. This analysis allows us to evaluate the stability of the flame front numerically depending on the conditions of the mixture.

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