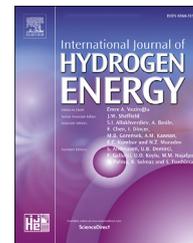




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Effects of Soret diffusion on the exergy losses in hydrogen laminar premixed flames

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HIGHLIGHTS

- The Soret diffusion role on the exergy loss in laminar premixed flames is studied.
- Hydrogen/air detailed reaction and the multicomponent transport models are adopted.
- Soret diffusion can appreciably affect the exergy loss contributions.
- Soret effect is not negligible especially when this affects laminar flame speed.
- The derivation of the Soret diffusion contribution to entropy generation is presented.

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ABSTRACT

The analysis of the exergy loss is an effective tool for evaluating second-law irreversibility in laminar flames. However, despite numerous studies underlining the importance of taking into account thermal diffusion in laminar flame studies, especially in hydrogen/air flames, this phenomenon is usually neglected in the exergy analysis of these flames. Therefore, this work investigates the effect of Soret diffusion on the exergy loss in laminar premixed flames for hydrogen/air mixtures using a detailed reaction mechanism and the multicomponent transport model. The study starts from conditions in which the importance of the Soret effect is well established in the scientific literature. It is found that, while the exergy losses directly due to the Soret effect are negligible, the Soret effect can appreciably affect the other exergy loss contributions and hence the total exergy loss. Hence, the Soret effect, unlike what has usually been assumed, is not negligible in flame calculations at least when this effect is known to affect laminar flame speed.

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Introduction

Energy production is undoubtedly one of the key factors in human development. However, traditional energy systems fail to meet the environmental and socioeconomic

requirements for sustainable human development. Therefore, a change in energy systems is needed both for satisfying the global energy demand increase and for tackling climate change. Developing new or improving existing energy systems requires addressing irreversibilities [1].

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An effective tool for evaluating the second-law irreversibility in energy conversion systems is the analysis of the exergy loss [2,3]. Indeed, many works in the scientific literature underline the importance of exergy analysis for the performance evaluation of energy systems (to deepen see the book authored by Dincer and Rosen [4]).

However, as shown in the review of Som and Datta [3], the greater amount of exergy loss in power generation systems is due to combustion phenomena. Therefore, several studies have been dedicated to investigating the irreversibilities in different combustion processes, see for instance: droplet combustion (e.g. [5–7]); spray combustion (e.g. [8,9]); coal/carbon combustion (e.g. [10,11]); laminar premixed flames (e.g. [2,12–15]); diffusion flames (e.g. [2,16]); constant volume combustion (e.g. [17,18]); triple flames (e.g. [19]). The entropy generation, i.e. the exergy loss, in these processes, is linked to four irreversible phenomena: chemical reactions, heat conduction, mass diffusion, and viscous dissipation [20].

Particularly, mass diffusion is an essential phenomenon in laminar flames. Indeed, it affects ignition, flame propagation, and extinction [21]. In a multi-component mixture, mass diffusion depends on three contributions associated with the mechanical driving forces and a contribution associated with the thermal driving force [22]. This latter contribution describes the chemical species diffusion under the influence of a temperature gradient; it is known as the Soret effect or thermal-diffusion effect. Usually, it is negligible because the thermal-diffusion coefficient is typically significantly smaller than the mass diffusion coefficient [22]. Nevertheless, it can be quantitatively significant at times and must be taken into account [23], especially if light or heavy fuels are considered [21]. The Soret effect drives light species toward hot regions of the flow and heavy species away from them [24]. Conversely, the companion effect, i.e. the energy flux due to a mass concentration gradient (also known as the Dufour effect) generally has a weak influence in laminar flame [23,25].

Since the pioneering study of Greenberg [26], the impact of the Soret effect on laminar flame has been widely studied (an in-depth review can be found in [23]), e.g.: García-Ybarra et al. [25] underlined that Soret mass diffusion cannot be neglected in the flame front dynamics studies; Ern and Giovangigli [24,27] showed the influence of thermal diffusion on hydrogen/air and methane/air (freely propagating and counterflow) flames; Rosner et al. [28] demonstrated quantitatively that, in air-fuel combustion systems especially in non-premixed ones, Soret effect is not confined to lightweight species (such as H, H₂, or CH₄), but it affects also heavy hydrocarbon fuel vapors and high molecular weight reaction intermediates (such as PAH molecules); Bongers and De Goeij [29], considering a one-dimensional adiabatic premixed flame with methane/air, methane/oxygen, hydrogen/air, and hydrogen/oxygen mixtures, obtained that neglecting thermal diffusion leads to significant errors in evaluating the flame burning velocity; Arias-Zugasti and Rosner [30] showed that in counterflow diffusion flames the Soret effect can introduce significant shifts in flame position and flame temperature; Grcar et al. [31] studied lean hydrogen/air premixed flames predicting hotter and significantly faster flames if the Soret effect is taken into account; Yang et al. [32,33] presented a study of Soret diffusion in hydrogen/air and n-butane/air

flames showing that this effect (especially the Soret effect of H) plays an important role in hydrogen/air flame speed while it almost has no influence on the butane/air flame speed; Xin et al. [34] investigated the influence of Soret diffusion on n-heptane/air flames (freely-propagating planar premixed flames, and counter-flow premixed and diffusion flames) underlining that in freely-propagating flames the net effect of the Soret diffusion (that primarily affects the chemical kinetics) is small while in the counter-flow cases its impact affects the flame temperature and flame burning intensity; Liang et al. [21] demonstrated that Soret diffusion reduces the laminar flame speed, at atmospheric pressure in premixed syngas/air flames, of unstretched planar flames and Markstein length of positively-stretched spherical flames; Liang et al. [35] reported that Soret diffusion leads to larger (smaller) minimum ignition energy (MIE) for relatively rich (lean) hydrogen/air mixtures; finally, Faghieh et al. [36] computed laminar flame speeds with and without considering Soret diffusion of a series of premixed spherical flames propagating at engine-relevant conditions (high temperature and pressures) with different fuels showing that Soret diffusion has significant influence for hydrogen/air and negligible effects for methane/air and iso-octane/air mixtures.

Despite these numerous studies underlining the importance of taking into account the thermal diffusion in laminar flame studies, especially when hydrogen/air flames are studied, this phenomenon is usually neglected in the exergy analysis of laminar premixed or diffusion flames. Therefore, a question arises: is it correct to neglect the Soret diffusion in the exergy analysis of hydrogen/air premixed laminar flames? This study aims to answer this question by computationally investigating the effect of Soret diffusion on the exergy loss in laminar premixed flames for hydrogen/air mixtures using a detailed reaction mechanism and transport data. Specifically, starting from conditions in which the importance of the Soret effect is well known, it has the purpose of verifying whether this effect is actually negligible with respect to the other exergy loss sources.

Methodology

Both Yang et al. [33] and Faghieh et al. [36] show that thermal diffusion may appreciably affect the laminar flame speed in premixed hydrogen/air flames. These results are adopted as the reference and the starting point for this study. Specifically, the results reported in Fig. 3 of Yang et al. [33] and in Fig. 2 of Faghieh et al. [36] are used as reference conditions for performing the exergy loss analysis.

The laminar flame speed of a premixed hydrogen/air mixture is calculated using the CHEMKIN software package [37]. The model used is the freely-propagating flame (a detailed mathematical formulation of this model can be found in [38]). The final computational domain is set to 0.12 m (120 mm) from -0.02 to 0.1 m, the adaptive grid controls based on, respectively, curvature and gradient are set to 0.005 and 0.002, the tolerance parameters are set to $1e-9$ for the absolute one and $1e-6$ for the relative one, and the maximum number of grid points allowed is set to 10,000. The transport properties are evaluated using the multicomponent transport model (see

for details Kee et al. [38]). In agreement with both Yang et al. [32] and Faghieh et al. [36], the detailed chemical mechanism consisting of 9 species and 20 reactions developed by Li et al. [39] is used to model hydrogen combustion.

The local entropy generation in laminar premixed flames, under the following assumptions:

1. Radiative heat transfer is negligible
2. Gas mixture is ideal
3. Pressure is constant throughout the flowfield
4. Dufour effect is negligible
5. Contribution due to viscous effects is negligible
6. Gravity is the only body force
7. Flow is steady, plane, and one-dimensional in the adopted frame of reference

can be quantitatively evaluated (see the Supplementary Material - Part A, for a detailed discussion of the topic) as:

$$\gamma_{\text{tot}} = \frac{\lambda}{T^2} \left(\frac{dT}{dx} \right)^2 + \rho R_m \sum_{k=1}^{N_s} \frac{D_{km}}{X_k} \left(\frac{dX_k}{dx} \right)^2 + \sum_{k=1}^{N_s} \frac{R_k D_k^T}{X_k T} \left(\frac{dT}{dx} \right) \left(\frac{dX_k}{dx} \right) - \frac{1}{T} \sum_{k=1}^{N_s} \sum_{j=1}^{N_r} \mu_k (\nu_{kj}^P - \nu_{kj}^R) r_j \quad (1)$$

In Eq. (1), four contributions can be distinguished.

- heat conduction

$$\gamma_{\text{hc}} = \frac{\lambda}{T^2} \left(\frac{dT}{dx} \right)^2$$

- mass diffusion

$$\gamma_{\text{diff}} = \rho R_m \sum_{k=1}^{N_s} \frac{D_{km}}{X_k} \left(\frac{dX_k}{dx} \right)^2$$

- mass diffusion by Soret effect

$$\gamma_{\text{diff, Soret}} = \frac{1}{T} \sum_{k=1}^{N_s} \frac{R_k D_k^T}{X_k} \left(\frac{dT}{dx} \right) \left(\frac{dX_k}{dx} \right)$$

- chemical reactions

$$\gamma_{\text{react}} = -\frac{1}{T} \sum_{k=1}^{N_s} \sum_{j=1}^{N_r} \mu_k (\nu_{kj}^P - \nu_{kj}^R) r_j$$

These quantities are evaluated, in order to investigate the relative importance of the Soret effect, in post-processing (from the flame numerical results) by using the Matlab® functions based on Cantera open-source suite [40] included as supplementary material (Part C).

The exergy losses are obtained using the Gouy-Stodola theorem [41]:

$$\dot{E}_{\text{loss}} = T_0 \gamma \quad (2)$$

Table 1 – Molar Fractions and standard chemical exergy at $P_0 = 101,325 \text{ Pa}$ and $T_0 = 298.15 \text{ K}$ of constituents of the reference environment.

Substance	Molar Fraction [%]	Molar Exergy [kJ/mol]
N ₂	75.67	0.72
O ₂	20.34	3.97
CO ₂	0.03	19.87
H ₂ O	3.03	9.49
He	0.00052	30.37
Ne	0.0018	27.19
Ar	0.92	11.69
Kr	0.000076	34.36

Here, the subscript 0 refers to the exergy reference environment that is assumed to be, in accordance with Moran et al. [42], an ideal gas mixture modeling Earth's atmosphere (Table 1 [43]) and γ refers to one of the previously defined contributions.

The exergy loss ratios are calculated as [14]:

$$E_{\text{loss}} = \frac{T_0 \int \gamma dx}{e_f} \quad (3)$$

where e_f is the initial chemical exergy carried by the mixture. It is defined as the product between the standard chemical exergy per unit mass of the unburned mixture (see the Supplementary Material - Part B for details), the density of the unburned mixture, and the laminar flame speed (being $\rho_u S_L$ the flow rate):

$$e_f = e_u \rho_u S_L \quad (4)$$

Results and discussion

Effect of Soret diffusion as a function of the equivalence ratio

Yang et al. [32,33] show that the Soret diffusion decreases the laminar flame speed in the entire range from lean to rich mixtures due to the downstream diffusion of H radicals (Fig. 1).

In order to verify whether the laminar flame model adopted and its parameters are the same as the reference work, a comparison between laminar flame speed data digitized from Yang et al. [33] and that computed for this study is carried out. Fig. 1 shows that there is a perfect match between computed and digitized data.

Computing the relative difference between the results obtained with and without the Soret effect:

$$\text{Relative difference}(S_{L,\text{Soret}}, S_{L,\text{noSoret}}) = \frac{S_{L,\text{Soret}} - S_{L,\text{noSoret}}}{0.5(S_{L,\text{Soret}} + S_{L,\text{noSoret}})}$$

allows for identifying the equivalence ratio in which this effect is more significant.

The relative difference is reported in Fig. 2. It results that the maximum effect of the Soret diffusion on the laminar flame speed is at an equivalence ratio of 0.7.

The entropy generation rates due to the four contributions previously listed are reported in Fig. 3 at $\phi = 0.7$, $P = 1 \text{ atm}$, and

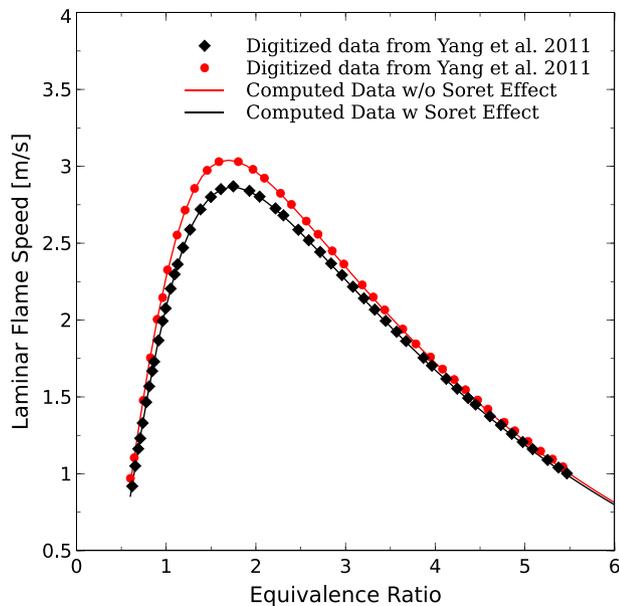


Fig. 1 – Laminar flame speed as function of equivalence ratio of hydrogen–air mixtures at $P = 1\text{atm}$ and $T_u = 300\text{K}$ with (black) and without (red) Soret effect. The symbols are the data digitized from Yang et al. [33] for comparison purposes.

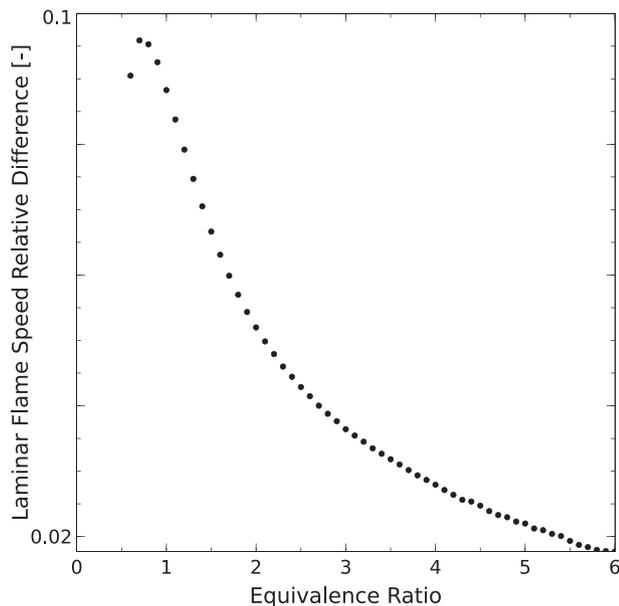


Fig. 2 – Relative difference between laminar flame speed computed with and without the Soret effect.

$T_u = 300\text{K}$. Despite the contribution due to the Soret effect sharply rises at the main reaction zone as similarly done by the other contributions, it remains an order of magnitude lower than the entropy generated by mass diffusion.

The low importance of the Soret effect in the entropy generation is confirmed by computing its relative weight with respect to the total mass diffusion (the sum of the mass

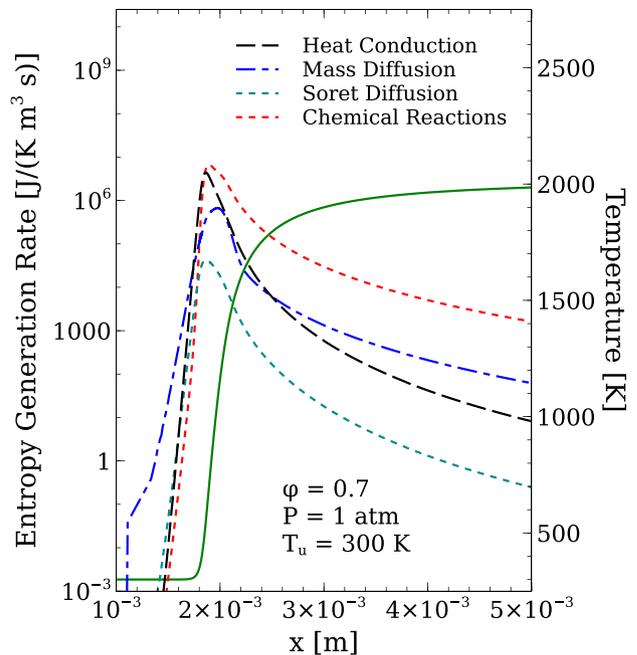


Fig. 3 – Entropy generation and temperature profile of premixed laminar flame at $\phi = 0.7$, $P = 1\text{atm}$, and $T_u = 300\text{K}$.

diffusion and Soret diffusion) and with respect to the total entropy generation (Fig. 4) by adopting the following relations:

$$RW_{\text{diff}} = \frac{\int \gamma_{\text{diff, Soret}} dx}{\int (\gamma_{\text{diff, Soret}} + \gamma_{\text{diff}}) dx} * 100$$

$$RW_{\text{tot}} = \frac{\int \gamma_{\text{diff, Soret}} dx}{\int (\gamma_{\text{diff, Soret}} + \gamma_{\text{diff}} + \gamma_{\text{hc}} + \gamma_{\text{react}}) dx} * 100$$

Clearly, being the relative weight of about 5.5% with respect to the entropy generated by mass diffusion and 0.42% with respect to the total entropy production, it appears that the entropy generated by Soret diffusion is negligible. However, an open question remains. Namely, it is needed to verify if neglecting the Soret diffusion in the laminar flame simulations may significantly affect the exergy loss due to other contributions. In order to carry out this verification, a comparison between the exergy loss ratios obtained with the Soret effect and without this phenomenon is presented in Fig. 5.

The results presented show that there is an appreciable effect due to the Soret diffusion on the exergy losses due to chemical reactions and heat conduction. For quantifying this effect, the relative errors between the exergy loss obtained with and without Soret diffusion are computed using the following relation:

$$\eta = \left| \frac{\dot{E}_{\text{loss}} - \dot{E}_{\text{loss, approx}}}{\dot{E}_{\text{loss}}} \right| * 100$$

where the subscript approx refers to results obtained neglecting the Soret effect. Neglecting the Soret diffusion leads

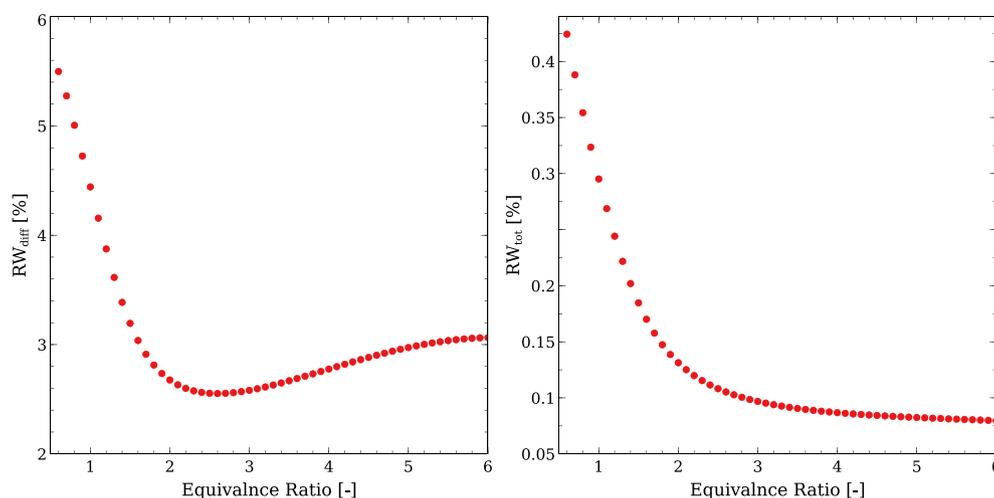


Fig. 4 – Relative weight of the entropy generated by the Soret effect with respect to the total mass diffusion (left) and the total entropy generation (right) at $P = 1\text{atm}$, and $T_u = 300\text{K}$.

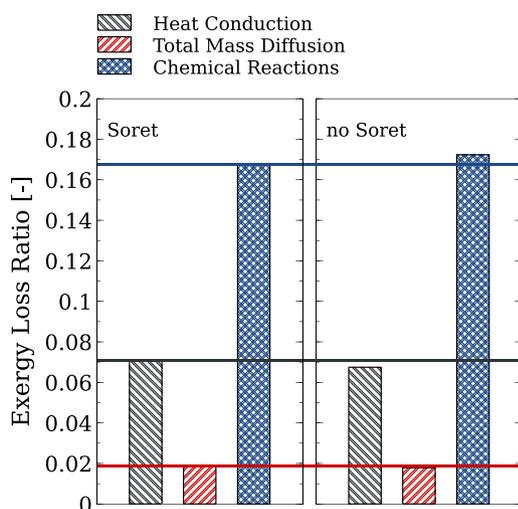


Fig. 5 – Comparison between results obtained with and without the Soret effect at $\phi = 0.7$, $P = 1\text{atm}$, and $T_u = 300\text{K}$.

to an overestimation of about 4.5% of the contribution due to heat conduction, 13.1% of that due to chemical reactions, and 3.8% of that due to total mass diffusion¹. Altogether the error on the total exergy loss (the sum of all the considered contributions) is about 10.1%. Therefore, neglecting the Soret effect significantly affects the exergy loss evaluation.

Effects of Soret diffusion under engine-relevant conditions

Faghii et al. [36] show that, for hydrogen/air mixtures, the Soret diffusion reduces the laminar flame speed up to around 10% in premixed flame under engine-relevant conditions (Fig. 6) mainly due to the Soret diffusion flux of H radicals and H₂ molecules.

Fig. 6 shows both the laminar flame speed results obtained by using the mixture-averaged transport model and the

¹ The sum of the contributions $\gamma_{\text{diff, Soret}}$ and γ_{Soret} (where the Soret effect was considered).

multicomponent formulation. The first results are computed only for validating the computation method because Faghii et al. [36] adopt the mixture-averaged transport model. The very small differences between the results obtained in this work and the results digitized from Faghii et al. [36] must be attributed to the different methods adopted to compute the laminar flame speed. Indeed, Faghii et al. [36], instead of using Chemkin for this purpose, developed an in-house code that takes advantage of Chemkin only for computing thermal and transport properties and reaction rates. However, in this work, to properly pursue its purposes, only the multicomponent formulation is considered to study the role of the Soret effect.

The relative difference between the results obtained with and without the Soret effect is reported in Fig. 7. Clearly, the Soret diffusion slightly decreases with pressure and temperature increases. The maximum effect of the Soret diffusion on the laminar flame speed is at $P = 1\text{atm}$, and $T_u = 350\text{K}$.

However, the relative weights of the entropy generated by the Soret effect with respect to the entropy generation by total mass diffusion (the sum of contributions due to the mass diffusion and Soret diffusion) and with respect to the total entropy generation (both shown in Fig. 8) indicate the need to investigate the Soret diffusion effects also at $P = 6\text{atm}$, and $T_u = 579.03\text{K}$ where RW_{diff} is maximum, and at $P = 19\text{atm}$, and $T_u = 792.30\text{K}$ where RW_{tot} is maximum.

The entropy generation due to the four entropy production mechanisms at the three identified conditions is reported in Fig. 9.

Clearly, these results show that the entropy generation contribution directly due to Soret diffusion is always negligible with respect to the other contributions. However, as done in the previous section, it is needed to verify if neglecting the Soret diffusion in the laminar flame simulations may significantly affect the exergy loss due to other contributions. The comparisons between the exergy loss ratios obtained with and without the Soret effect are presented in Fig. 10 for the three conditions identified.

It results that there is an appreciable effect due to the Soret diffusion on all the other contributions to the exergy loss. The

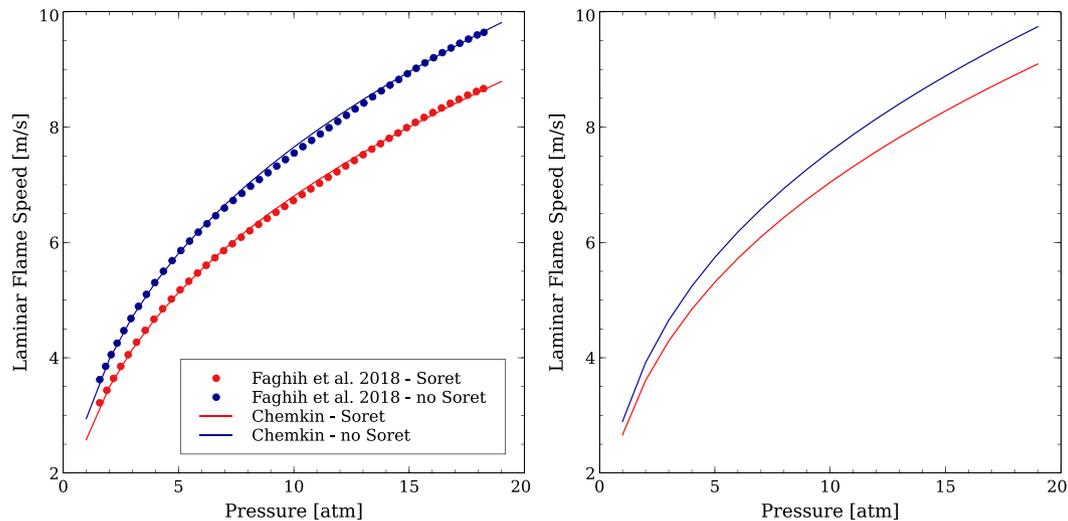


Fig. 6 – Laminar flame speed of hydrogen–air mixtures as a function of pressure at $\varphi = 1$ with (black) and without (red) Soret effect: at left the results obtained by mixture averaged transport model, at right that obtained by the more accurate multicomponent formulation. The temperature of the unburned mixture changes with pressure following the isentropic compression relationship with the initial values of $P = 1\text{atm}$, and $T_u = 350\text{K}$. The symbols are the data digitized from Faghih et al. [36] for comparison purposes.

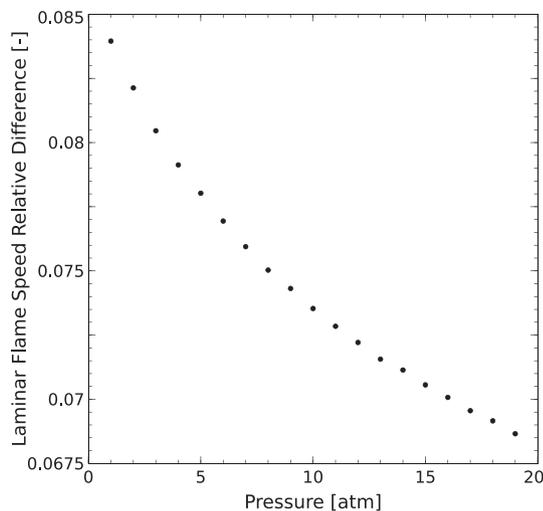


Fig. 7 – Relative difference between laminar flame speed computed with and without the Soret effect.

relative error that would be made in neglecting the Soret effect is summarized in Table 2.

The reported results show that neglecting the Soret effect significantly affects the exergy loss due to the chemical reactions while the effect on the contributions due to other exergy loss sources is negligible. However, the inclusion of the Soret diffusion in the laminar flame model, as in the previous study case, leads to a significant change in the estimated value of the total exergy loss.

Indirect effect of Soret diffusion

According to the reported results, the exergy losses directly due to the Soret effect ($\dot{E}_{\text{loss,diff,Soret}}$) are always negligible with respect to the other exergy loss sources. However, neglecting the Soret diffusion affects the evaluation of the other contributions to the exergy loss especially the one due to the chemical reactions. Therefore, there is an indirect effect of the Soret diffusion on others exergy loss contributions.

An explanation of this indirect effect requires an examination of the distribution of the H radicals (as indicated by Yang et al. [32]), for the range 0–7 mm reported in Fig. 11, and of entropy generation profiles, for the range 1.5–3 mm shown in Fig. 12. For deepening this effect, the conditions of the study case reported in section 3.1 ($\varphi = 0.7$, $P = 1\text{atm}$, and $T_u = 300\text{K}$) have been adopted because this study case is the worst-case scenario (total entropy loss error of 10.1%). The results for the others study cases are qualitatively similar.

Fig. 11 shows that there is, when the Soret effect is taken into account, a reduction in the concentration of H. Fig. 12 shows that neglecting the Soret diffusion leads overall to an overestimation of the exergy loss. However, observing the entropy generation rate profile due to the total mass diffusion it is possible to underline that locally the entropy generation rate computed by considering the Soret effect is greater than that obtained neglecting this phenomenon approximately in the range spanning from 1.5 to 1.85 mm. These results are in agreement with those reported by Yang et al. [32]. The role of Soret diffusion on H radicals is to move them from the reaction zone toward the downstream direction reducing their

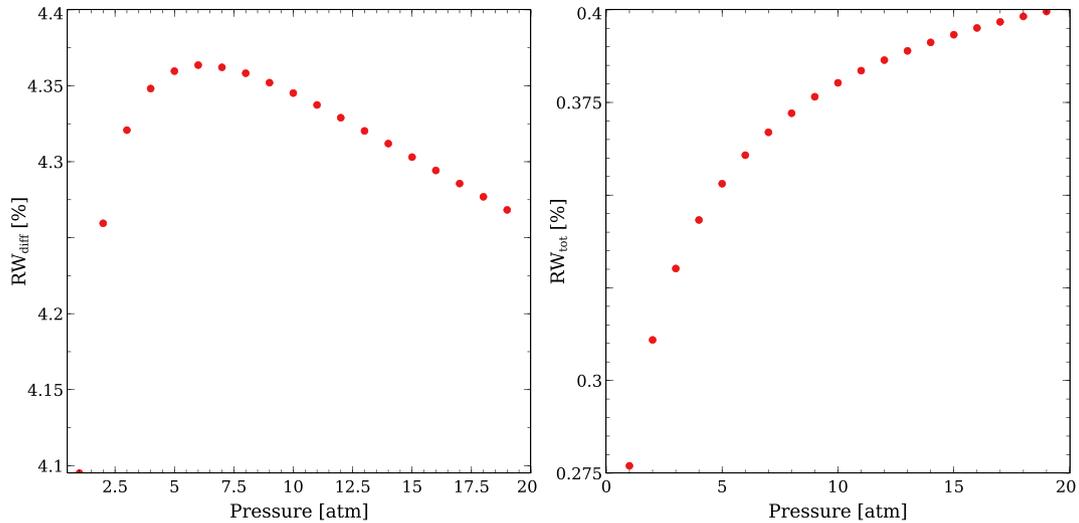


Fig. 8 – Relative weight of the entropy generated by the Soret effect with respect to the entropy production by total mass diffusion (left) and the total entropy generation (right) at $\phi = 1$. The temperature of the unburned mixture changes with pressure following the isentropic compression relationship with the initial values of $P = 1\text{atm}$, and $T_u = 350\text{K}$.

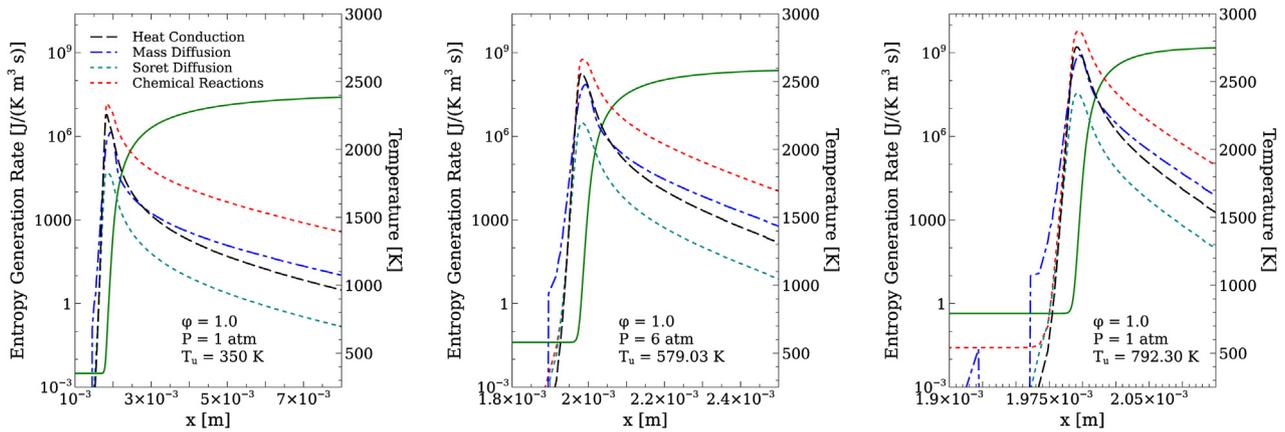


Fig. 9 – Entropy generation and temperature profile of premixed laminar flame at: $\phi = 1.0$, $P = 1\text{atm}$, and $T_u = 350\text{K}$ (left); $\phi = 1.0$, $P = 6\text{atm}$, and $T_u = 579.03\text{K}$ (center); $\phi = 1.0$, $P = 19\text{atm}$, and $T_u = 792.30\text{K}$ (right).

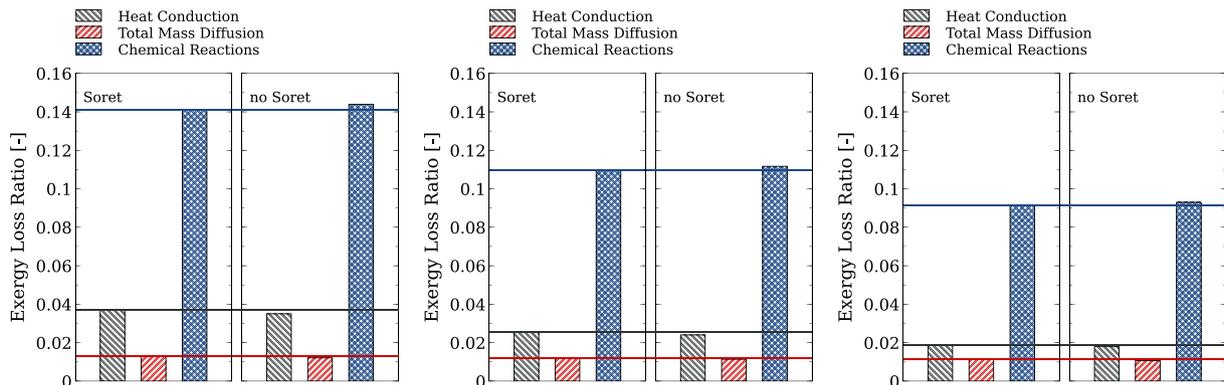
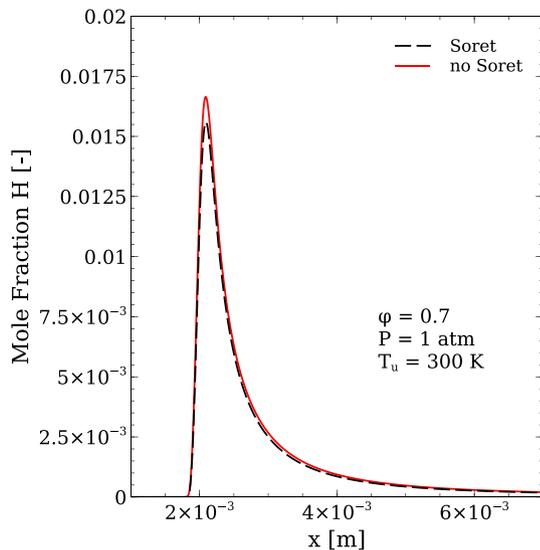


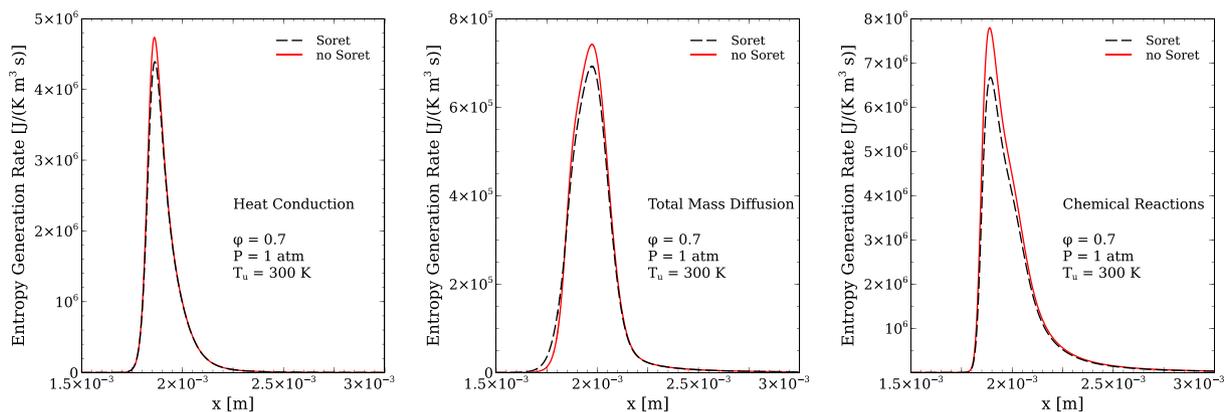
Fig. 10 – Comparison between results obtained with and without Soret effect at: $\phi = 1.0$, $P = 1\text{atm}$, and $T_u = 350\text{K}$ (left); $\phi = 1.0$, $P = 6\text{atm}$, and $T_u = 579.03\text{K}$ (center); $\phi = 1.0$, $P = 19\text{atm}$, and $T_u = 792.30\text{K}$ (right).

Table 2 – Relative error in neglecting the Soret effect.

Pressure - Temperature	P = 1atm - T _u = 350K	P = 6atm - T _u = 579.03K	P = 19atm - T _u = 792.30K
Heat Conduction	3.0%	2.1%	1.9%
Total Mass Diffusion	1.9%	0.6%	0.3%
Chemical Reactions	10.9%	9.7%	9.0%
Total	8.8%	7.6%	7.1%

**Fig. 11 – Mole fractions of H for the laminar premixed flame at $\phi = 0.7$, $P = 1\text{atm}$, and $T_u = 300\text{K}$, allowing no Soret diffusion and Soret diffusion for all species.**

concentration. This effect awakens the reaction intensity, namely, it reduces reactions rates, temperature gradient, and mole fraction gradients and consequently the entropy generation rates (that are functions of these quantities) and, therefore, the exergy losses.

**Fig. 12 – Entropy generation profiles for the laminar premixed flame at $\phi = 0.7$, $P = 1\text{atm}$, and $T_u = 300\text{K}$, allowing no Soret diffusion and Soret diffusion for all species.**

Conclusions

The present study computationally investigates the effect of Soret diffusion on the exergy loss in laminar premixed flames using a detailed reaction mechanism and the multicomponent transport model.

The investigation started from the results of Yang et al. [33] and Faghieh et al. [36]. Namely, the role of the Soret effect is studied both at atmospheric conditions by varying the equivalence ratio and under engine-relevant conditions, i.e. under conditions where it was demonstrated that thermal diffusion appreciably affects the laminar flame speed in pre-mixed hydrogen/air flames.

The results obtained lead to the following conclusions:

- the exergy losses directly due to the Soret effect ($\dot{E}_{\text{loss,diff,Soret}}$) are always negligible with respect to the other contributions;
- there is an indirect effect of the Soret diffusion on others exergy loss contributions;
- neglecting thermal diffusion leads to an overestimation (relative error) of the total exergy loss that stood in the range of 7.1%–10.1% (values comparable to errors on laminar flame speed evaluation reported in the literature).

Hence, the Soret effect, unlike what has been usually assumed in previous studies, is not negligible in evaluating the exergy loss in premixed laminar flames at least when this effect is known to affect laminar flame speed.

Nomenclature

\dot{E}_{loss}	Exergy loss rate
η	Relative error
γ	Entropy production
λ	Thermal conductivity

μ_k	Chemical potential of the k-th species
ν_{kn}^P	Stoichiometric coefficients of products
ν_{kn}^R	Stoichiometric coefficients of reactants
ρ	Density of the mixture
ρ_u	Density of the unburned mixture
φ	Equivalence ratio
D_k^T	Thermal diffusion coefficient of the k-th species
D_{km}	Equivalent Fickian diffusion coefficient
e_f	Initial chemical exergy carried by the mixture
e_u	Standard chemical exergy per unit mass of the unburned mixture
E_{loss}	Exergy loss ratio
N_r	Number of chemical reactions
N_s	Number of chemical species
P	Pressure
P_0	Pressure of the reference environment
r_j	Net rate of progress of the j-th reaction
R_k	Gas constant of the k-th species
R_m	Mixture gas constant
RW_{diff}	Relative weight of the contribution in the entropy generation due to Soret effect with respect to that due to the total mass diffusion
RW_{tot}	Relative weight of the contribution in the entropy generation due to Soret effect with respect to the total entropy generation
S_L	Laminar flame speed
T	Absolute temperature
T_0	Temperature of the reference environment
T_u	Temperature of the unburned mixture
X_k	Mole fraction of the k-th species

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.

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.ijhydene.2023.03.404>.

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