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# Lewis number and preferential diffusion effects in lean hydrogen–air highly turbulent flames

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**Note:** This paper is part of the special topic, Development and Validation of Models for Turbulent Reacting Flows.

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## ABSTRACT

Unsteady three-dimensional direct numerical simulations of highly turbulent, complex-chemistry, lean hydrogen–air flames were performed by changing the equivalence ratio  $\phi$ , root mean square velocity  $u'$ , and turbulence length scale  $L$ . For each set of  $\{\phi, u', L\}$ , to explore the influence of molecular transport coefficients on the turbulent burning velocity  $U_T$ , four cases were designed: (i) mixture-averaged diffusivities; (ii) diffusivities equal to the heat diffusivity  $\kappa$  of the mixture for all species; (iii) mixture-averaged diffusivities for all species with the exception of  $O_2$ , whose diffusivity was equal to the diffusivity  $D_{H_2}$  of  $H_2$  to suppress preferential diffusion effects; and (iv) mixture-averaged diffusivities multiplied with  $\kappa/D_{H_2}$  to suppress Lewis number effects but retain preferential diffusion effects. The computed results show a significant increase in  $U_T$  due to differences in molecular transport coefficients even at Karlovitz number  $Ka$  as large as 565. The increase is documented in cases (i) and (iii) but is not observed in case (iv)—indicating that this phenomenon is controlled by Lewis number effects, whereas preferential diffusion effects play a minor role. The phenomenon is more pronounced in leaner flames, with all other things being equal. While the temperature profiles  $\langle T|c_F \rangle(c_F)$  conditionally averaged at the local value of the combustion progress variable  $c_F$  and sampled from the entire flame brushes are not sensitive to variations in molecular transport coefficients at high  $Ka$ , the  $\langle T|c_F \rangle(c_F)$ -profiles sampled from the leading edges of the same flame brushes show significant increase in the local temperature in cases (i) and (iii) characterized by a low Lewis number.

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## I. INTRODUCTION

Due to the threat of global warming, there has been a rapidly growing interest in the conversion of energy bond in renewable carbon-free fuels such as  $H_2$ . From the combustion perspective, to facilitate transition to carbon-free energetics and transport, there is an urgent need for developing models capable of predicting major characteristics of lean turbulent burning of  $H_2$  or fuel blends that contain molecular hydrogen ( $CH_4/H_2$ ,  $NH_3/H_2$ , or syngas). While significant progress has recently been made in understanding both the influence of turbulence on a premixed flame<sup>1–6</sup> and the influence of combustion-induced thermal expansion on turbulence,<sup>7–12</sup> a crucial unresolved challenge associated with lean turbulent burning of  $H_2$  consists of predicting the abnormally high turbulent flame speeds well documented in

experiments with lean  $H_2$ –air, syngas–air, and  $NH_3/H_2$ –air mixtures, see a review article<sup>13</sup> and more recent papers.<sup>14–19</sup>

This phenomenon is commonly attributed to local changes in the equivalence ratio and temperature due to the imbalance of (i) molecular fluxes of fuel and oxygen or (ii) molecular fluxes of reactants and heat to/from the reaction zones curved and strained by turbulent eddies.<sup>13,20,21</sup> The former and latter mechanisms are known as preferential diffusion and Lewis number effects, respectively. In the case of a laminar flow and single-step chemistry, activation energy asymptotic theories describe such effects in weakly stretched<sup>22,23</sup> and slowly varying<sup>24,25</sup> flames of an arbitrary configuration or in critically strained counter-flow<sup>20,26</sup> flames. Some of these theories<sup>24,25</sup> predict that Lewis number effects overwhelm preferential diffusion effects if the mixture

composition is far from stoichiometric. Other theories<sup>20</sup> imply the importance of preferential diffusion effects also. When discussing molecular transport effects in complex-chemistry turbulent flames, both Lewis number and preferential effects are often considered. Certain models of turbulent combustion highlight the latter effects,<sup>20,27</sup> whereas instantaneous two-dimensional images of hydrogen mass fraction, temperature, and fuel consumption rate, obtained by Aspden<sup>28</sup> from a single moderately turbulent flame invoking different models of molecular transport, indicate that the preferential diffusion effects are of minor importance when compared to the Lewis number effects. However, changes in turbulent burning velocity caused by these two effects have not yet been compared; this work aimed initially at filling this knowledge gap by analyzing results of a specially designed set of direct numerical simulations (DNSs). Since other results obtained by analyzing the DNS data appear to be of interest, some of them will also be presented in the following.

In Sec. II, the DNS attributes are briefly reported. Numerical results are discussed in Sec. III, followed by conclusions.

## II. DNS ATTRIBUTES

Since the DNS attributes have already been discussed in detail elsewhere,<sup>29–31</sup> only a brief summary of the simulations is provided below. Statistically planar and one-dimensional, unconfined, lean H<sub>2</sub>–air turbulent flames were simulated using a detailed chemical mechanism (nine species, 22 reactions) by Kéromnès *et al.*<sup>32</sup> Unsteady three-dimensional continuity, Navier–Stokes, and transport equations written in the low-Mach-number approximation were numerically integrated by adopting the solver *DINO*<sup>33</sup> in a rectangular computational domain of  $\Lambda \times 16\Lambda \times \Lambda$ . The domain was covered with a uniform Cartesian mesh of  $N_x \times 16N_x \times N_x$  cells. Along the streamwise  $y$ -direction, the inflow and outflow boundary conditions were set. Other boundary conditions were periodic.

In a layer of  $0.5\Lambda \leq y \leq 8\Lambda$ , the linear forcing method<sup>34,35</sup> was applied to generate turbulence. The turbulence characteristics are reported elsewhere.<sup>29</sup> In a single case C, one more DNS was run by switching off turbulence generation, i.e., the turbulence decayed in time, with all other things being equal. As discussed elsewhere,<sup>29,30</sup> this change of turbulence evolution did not change the major effects of small-scale turbulence on the local burning.

The simulation conditions are reported in Table I, where  $\phi$  is the equivalence ratio;  $S_L$  and  $\delta_L^T = (T_b - T_u)/\max\{|dT/dy|\}$  are the laminar flame speed and thickness, respectively, pre-computed using the same chemical mechanism<sup>32</sup> and code *Cantera*<sup>36</sup> under room conditions;  $u'$  and  $L$  are the root mean square turbulent velocity and integral length scale, respectively;  $Da = \tau_t/\tau_f$  is the Damköhler number;  $Ka = (u'/S_L)^{3/2}(\delta_L^T/L)^{1/2}$  is the Karlovitz number;  $Re_t = u'L/\nu_u$  is the turbulent Reynolds number;  $T$  designates the temperature;  $\tau_t = L/u'$  and  $\tau_f = \delta_L^T/S_L$  are the turbulence time scale and the laminar flame time scale, respectively;  $\nu_u$  is the kinematic viscosity of unburned mixture;  $\eta = LRe_t^{-3/4}$  is the Kolmogorov length scale;  $\Delta x$  is the mesh step; and the subscripts  $u$  and  $b$  designate unburned and burned mixtures, respectively. Reported in the two right-most columns are time-averaged values of dimensional and normalized burning velocity evaluated as follows:

$$U_T^F(t) = \frac{1}{(\rho Y_{H_2})_u \Lambda^2} \iiint_{\Omega} |\dot{\omega}_{H_2}|(\mathbf{x}, t) d\mathbf{x}. \quad (1)$$

Here,  $\rho$  is the density,  $Y_{H_2}$  is the fuel mass fraction,  $\dot{\omega}_{H_2}$  is the fuel consumption rate, and  $\Omega$  designates the computational domain.

DNS data obtained in cases C and C1 were analyzed in our earlier papers.<sup>29–31</sup> New cases D and D1, E and E1, and F and F1 were designed to explore the Lewis number and preferential diffusion effects under various equivalence ratios,  $u'/S_L$ , and  $L/\delta_L^T$ . First, flames C and D propagate in the statistically same turbulence regime but are

TABLE I. Major characteristics of simulated flames.

Case	$\phi$	$S_L$ , m/s	$\delta_L^T$ , mm	$\frac{u'}{S_L}$	$\frac{L}{\delta_L^T}$	$Da$	$Ka$	$Re_t$	$\frac{\Delta x}{L}$	$\frac{\Delta x}{\eta}$	$N_x$	$\Lambda$ , mm	$\overline{U_T^F(t)}$ m/s	$\frac{\overline{U_T^F(t)}}{S_L}$
C	0.5	0.58	0.41	11.2	1.10	0.10	33.0	158	0.041	1.85	128	2.4	5.14	8.86
C/O <sub>2</sub>	0.5	0.59	0.42	11.1	1.10	0.10	35.5	158	0.041	1.85	128	2.4	5.17	8.82
C/T	0.5	0.80	0.30	8.2	1.50	0.19	18.8	158	0.041	1.85	128	2.4	2.55	3.20
C1	0.5	0.78	0.29	8.3	1.60	0.19	19.0	158	0.041	1.85	128	2.4	3.32	4.26
D	0.35	0.12	0.92	54.1	0.49	0.017	565	160	0.041	1.85	128	2.4	1.78	14.9
D/O <sub>2</sub>	0.35	0.13	0.83	49.4	0.52	0.011	481	160	0.041	1.85	128	2.4	2.03	15.4
D/T	0.35	0.29	0.43	21.9	1.05	0.05	100	160	0.041	1.85	128	2.4	1.02	3.42
D1	0.35	0.30	0.43	21.6	1.10	0.05	97	160	0.041	1.85	128	2.4	1.08	3.61
E	0.35	0.12	0.92	11.2	0.50	0.04	53.2	33	0.082	1.13	64	2.4	1.49	12.4
E/O <sub>2</sub>	0.35	0.13	0.83	10.2	0.52	0.05	45.2	33	0.082	1.13	64	2.4	1.72	13.1
E/T	0.35	0.29	0.43	4.5	1.02	0.23	9.4	33	0.082	1.13	64	2.4	0.48	1.6
E1	0.35	0.30	0.43	4.5	1.07	0.24	9.1	33	0.082	1.13	64	2.4	0.66	2.2
F	0.35	0.12	0.92	11.2	1.15	0.10	34.8	77	0.041	1.07	128	5.6	2.70	22.5
F/O <sub>2</sub>	0.35	0.13	0.83	10.2	1.22	0.12	29.6	77	0.041	1.07	128	5.6	2.70	20.5
F/T	0.35	0.29	0.43	4.5	2.45	0.54	6.14	77	0.041	1.07	128	5.6	1.04	3.5
F1	0.35	0.30	0.43	4.5	2.50	0.56	5.96	77	0.041	1.07	128	5.6	1.37	4.5

characterized by different  $\phi$  and, hence, by different  $S_L$ ,  $\delta_L^T$ , or  $\tau_f$ . Accordingly, the values of  $u'/S_L$ ,  $L/\delta_L^T$ ,  $Da$ , or  $Ka$  are also different for the two flames. Second, flames D and E are characterized by different  $u'$  (and, hence, different  $Da$  or  $Ka$ ), but the same  $\phi$  or  $L/\delta_L^T$ . In addition, flames C and E are characterized by approximately equal ratios of  $u'/S_L$ , but different  $\phi$ ,  $L/\delta_L^T$ ,  $Da$ , or  $Ka$ . Third, in case F, the domain width  $\Lambda$  and the length scale  $L$  are increased for the values of  $u'/S_L$ ,  $L/\delta_L^T$ ,  $Da$ , or  $Ka$  to be approximately equal in cases C and F. Thus, the major difference between these two cases consists of the equivalence ratio. Among the eight aforementioned cases, flame D is characterized by the lowest  $Da$  and the highest  $Ka$ .

The sole difference between cases  $\mathcal{L}$  and  $\mathcal{L}1$ , where  $\mathcal{L}$  subsumes a capital letter (C, D, E, or F), consists of changing the mixture-averaged molecular diffusivities  $D_k \neq \kappa$  (cases  $\mathcal{L}$ ) to  $D_k = \kappa$  for all species  $k$  (cases  $\mathcal{L}1$ ). Here,  $\kappa$  is the molecular heat diffusivity of the mixture. In cases  $\mathcal{L}1$ , the computed  $S_L$  is larger, in line with the theory of laminar premixed flames.<sup>26</sup> Cases  $\mathcal{L}/O_2$  and  $\mathcal{L}/T$  were designed to compare the magnitudes of the Lewis number and preferential diffusion effects. More specifically, to suppress the latter effects in cases  $\mathcal{L}/O_2$ , cases  $\mathcal{L}$  were modified by setting  $D_{O_2} = D_{H_2}$ , with all other input parameters being unchanged. To suppress the former effects in case  $\mathcal{L}/T$ , cases  $\mathcal{L}$  were modified by multiplying the molecular diffusivities of all species with  $\kappa/D_{H_2}$ . For the studied

lean  $H_2$ -air mixtures, the Lewis number  $Le = \kappa/D_{H_2} = 0.39$  in case C and 0.36 in cases D, E, F. Thus, the preferential diffusion mechanism is eliminated in flames  $\mathcal{L}/O_2$ , which are still subject to Lewis number effects, whereas the latter effects are eliminated in flames  $\mathcal{L}/T$ , which are still subject to preferential diffusion.

Each turbulent flame was initialized by embedding a pre-computed steady, planar, one-dimensional laminar flame solution at  $y = 8N_x$ . When necessary, the mean inlet velocity was manually changed to keep the flame within the forced-flow subdomain. Statistics was sampled after a transition stage, whose duration was equal to  $3\tau_t$  (case F),  $5\tau_t$  (other F-flames),  $15\tau_t$  (cases C, C/T, and C1), or  $10\tau_t$  (all other flames). When processing the DNS data, conventional or conditional averaging was applied across the transverse planes  $y = \text{const}$ . For an arbitrary quantity  $q$ , its instantaneous transverse-averaged value is designated with  $\langle q \rangle(y, t)$  in the following, whereas overbar refers to time averaging, performed over at least  $25\tau_t$ .

The combustion progress variable is defined using the fuel mass fraction, i.e.,  $c_F = (Y_{H_2,u} - Y_{H_2})/Y_{H_2,u}$ , and the local equivalence ratio is equal to

$$\phi = \frac{1}{2} \frac{2X_{H_2} + 2X_{H_2O} + X_H + X_{OH} + X_{HO_2} + 2X_{H_2O_2}}{2X_{O_2} + X_{H_2O} + X_O + X_{OH} + 2X_{HO_2} + 2X_{H_2O_2}}, \quad (2)$$

where  $X_S$  is the mole fraction of species S.

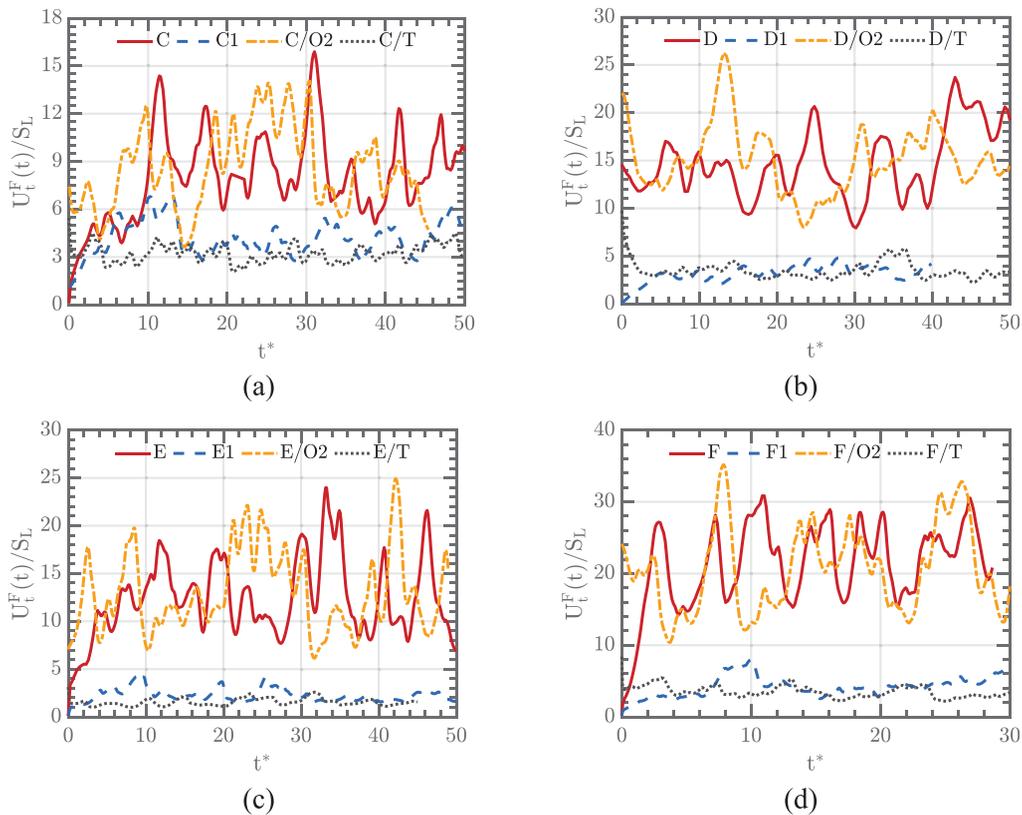
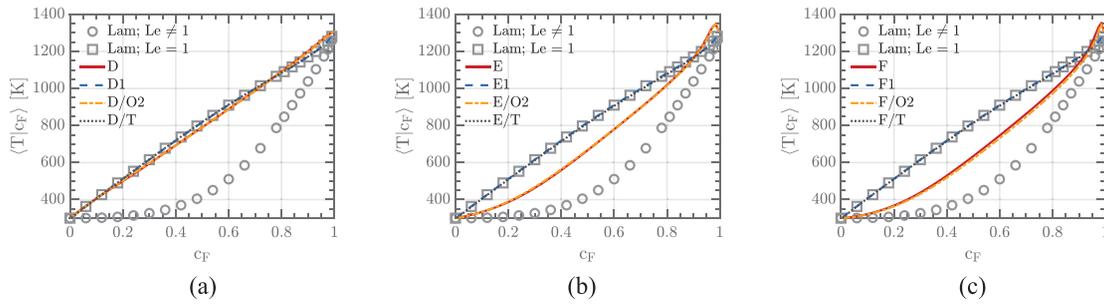


FIG. 1. Dependencies of the normalized turbulent burning velocities  $U_t^F(t)/S_L$  on the normalized time  $t^* = t/\tau_t$ , computed in (a) C, (b) D, (c) E, and (d) F sets of flames. Case names are reported in legends.



**FIG. 2.** Conditioned temperatures extracted from entire flame brushes in cases  $\mathcal{L}$  (red solid lines),  $\mathcal{L}/O_2$  (orange dotted-dashed lines),  $\mathcal{L}/T$  (black dotted lines), and  $\mathcal{L}1$  (blue dashed lines). The circles and squares show  $T_{c_F}$  obtained from low Lewis number and equidiffusive unperturbed laminar flames, respectively, corresponding to cases D–F and D1–F1, respectively. (a) D, (b) E, and (c) F sets of flames.

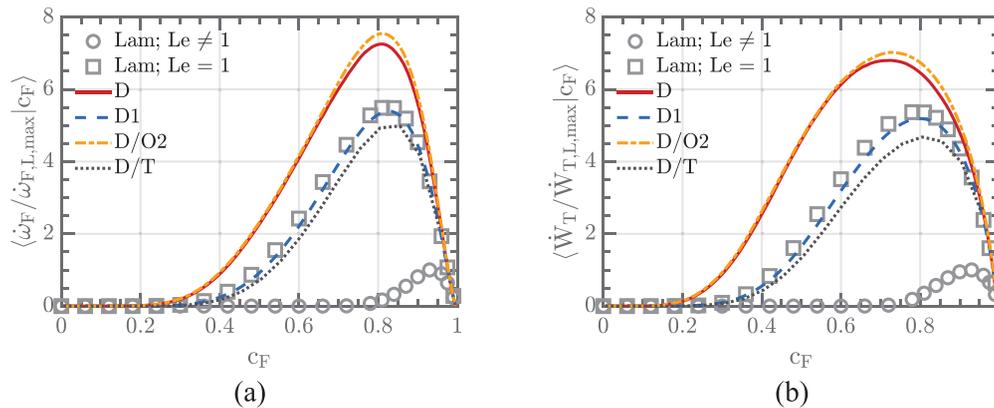
**III. RESULTS AND DISCUSSION**

Figure 1 shows the dependencies of the normalized turbulent burning velocities  $U_T^F(t)/S_L$  on the normalized time  $t^* = t/\tau_t$ , with the time-averaged burning velocities being reported in Table I. The following trends are worth emphasizing.

First, a comparison of the curves plotted in red solid and blue dashed lines shows that an increase in the turbulent burning rate due to differences in molecular transport coefficients is well pronounced in all sets of flames. For instance, the ratio  $\mathbb{R} = \left(\overline{U_T^F}/S_L\right)_{\mathcal{L}} / \left(\overline{U_T^F}/S_L\right)_{\mathcal{L}1}$  of the normalized turbulent burning velocities computed in low Lewis number cases  $\mathcal{L}$  and equidiffusive cases  $\mathcal{L}1$  is equal to 2.1, 4.1, 5.7, and 5.0 for C, D, E, and F sets of flames, respectively. The effect is significant even at  $Ka$  as large as 565 (case D), while  $\mathbb{R}$  decreases from 5.7 to 4.1 with an increase in  $u'/S_L$  from 11 (case E) to 54 (case D). At the same time,  $\mathbb{R}$  is larger at  $Ka = 53$  (case E) when compared to  $Ka = 35$  (case F). Moreover,  $\mathbb{R}$  is significantly larger in a leaner flame F than in flame C despite the major non-dimensional characteristics ( $u'/S_L$ ,  $L/\delta_L^T$ ,  $Da$ , and  $Ka$ ) of the two flames being almost equal. Even the dimensional values of  $\overline{U_T^F}$  are significantly larger in cases  $\mathcal{L}$  than in equidiffusive cases  $\mathcal{L}1$  despite the opposite trend being observed for  $S_L$ .

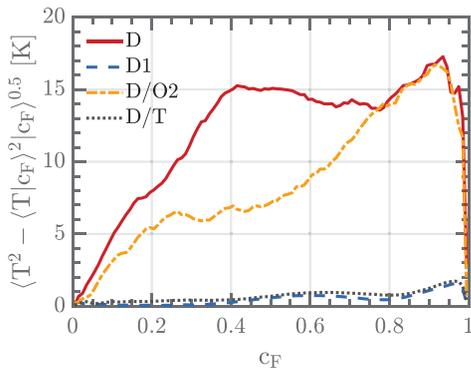
Second, a comparison of the curves plotted in orange dotted-dashed lines and black dotted lines with the curves plotted in red solid lines shows that, in cases  $\mathcal{L}/O_2$ ,  $U_T^F/S_L$  is close to large  $U_T^F/S_L$  in cases  $\mathcal{L}$  and is significantly larger than  $U_T^F/S_L$  in cases  $\mathcal{L}/T$ . Moreover, in the latter cases,  $U_T^F/S_L$  is comparable with low  $U_T^F/S_L$  in cases  $\mathcal{L}1$ , cf. curves plotted in black dotted and blue dashed lines. The same trends hold for the time-averaged burning velocity, see Table I. Thus, in all four low Lewis number flames  $\mathcal{L}$ , a significant increase in  $U_T^F/S_L$  when compared to equidiffusive flames  $\mathcal{L}1$  is controlled by the Lewis number effects. Preferential diffusion effects play a minor (if any) role.

On the contrary, Fig. 2(a) does not show an increase in conditioned temperatures  $\langle T_{c_F} \rangle$  extracted from entire flame brushes in cases D and D/O<sub>2</sub> when compared to cases D1 and D/T. Moreover, all four conditioned profiles of  $\langle T_{c_F} \rangle$ , extracted from the turbulent flames, are very close to a profile of  $T_{c_F}$  obtained from the equidiffusive unperturbed laminar flame (squares), corresponding to cases D1–F1. These results computed at the highest  $Ka$ , see Table I, are in line with earlier DNS findings,<sup>37–40</sup> which indicated that an increase in  $Ka$  resulted in vanishing sensitivity of the conditioned profiles of species concentrations and temperature to differences in molecular transport coefficients. However, Fig. 2(a) appears to be inconsistent with Fig. 1(b) at first glance.



**FIG. 3.** Conditioned (a) fuel consumption and (b) heat release rates sampled from entire flame brushes and normalized using the highest rates in the low  $Le$  laminar flame. D-set of cases. Line legends are explained in caption to Fig. 2. The circles and squares show the profiles obtained from the laminar counterparts of flames D and D1, respectively.

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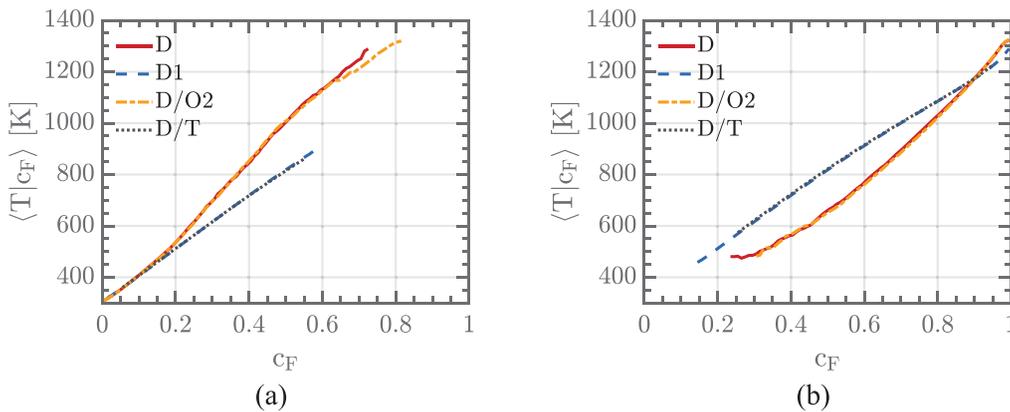
**FIG. 4.** Conditioned profiles of root mean square temperature  $\langle T^2 - \langle T|_{c_F} \rangle^2 |_{c_F} \rangle^{0.5}$  sampled from entire flame brushes in D-set of cases. Line legends are explained in caption to Fig. 2.

Furthermore, Figs. 2(b) and 2(c) show a decrease in  $\langle T|_{c_F} \rangle (c_F < 0.9)$  in flames E and E/O<sub>2</sub> or F and F/O<sub>2</sub> when compared to flames E1 and E/T or F1 and F/T, respectively, whereas Figs. 1(c) and 1(d) imply the opposite trend. The latter ( $\mathcal{L}/T$  and  $\mathcal{L}1$ ) conditioned

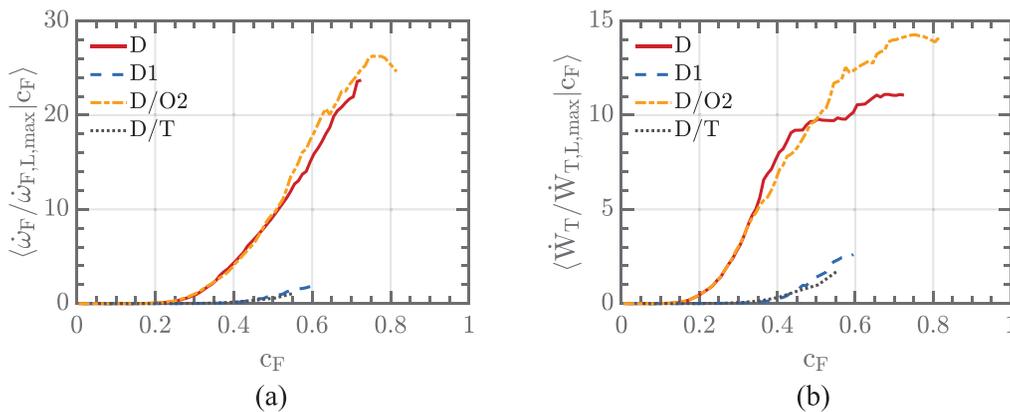
temperature profiles are again very close to  $T(c_F)$  obtained from the equidiffusive unperturbed laminar flame (squares), whereas the former ( $\mathcal{L}$  and  $\mathcal{L}/O_2$ ) profiles lie between  $T(c_F)$  obtained from the equidiffusive (squares) and low Lewis number (circles) laminar flames. Since flames E and F are characterized by  $Ka$  lower than in case D, these results further illustrate (in line with earlier studies<sup>37–40</sup>) that a sufficiently high  $Ka$  should be reached to suppress the sensitivity of conditioned profiles of temperature to differences in molecular transport coefficients.

The apparent inconsistency between the results plotted in Figs. 1 and 2 might be attributed to two effects. First, Fig. 3 shows that the conditioned fuel consumption and heat release rates sampled from the entire flame brushes are substantially higher in cases D and D/O<sub>2</sub> than in cases D1 and D/T despite approximately the same profiles  $\langle T|_{c_F} \rangle (c_F)$  reported in Fig. 2(a). This difference in the rates might be attributed to their highly non-linear dependencies on  $T$  and to different magnitudes of fluctuations of the local temperature in the studied flames. Figure 4 does show differences in the root mean square conditioned temperatures  $\langle T^2 - \langle T|_{c_F} \rangle^2 |_{c_F} \rangle^{1/2}$ , but the magnitude of these differences appears to be too low to explain the rate differences in Fig. 3.

Second, it is worth stressing that the results reported in Figs. 2–4 have been sampled from entire flame brushes, whereas the



**FIG. 5.** Conditioned temperatures extracted from the (a) leading and (b) trailing edges of flame brushes. Line legends are explained in caption to Fig. 2. D-set of flames.



**FIG. 6.** Normalized conditioned (a) fuel consumption and (b) heat release rates sampled from the leading edges of flame brushes. Line legends are explained in caption to Fig. 2. D-set of flames.

conditioned profiles sampled from the leading or trailing edges of these flame brushes show very different behavior. For instance, Figs. 5(a) and 5(b) report the conditioned profiles  $\langle T|_{c_F}(c_F)$  sampled from layers characterized by  $\langle c_F \rangle(y, t) = 0.1 \pm 0.005$  (leading edge) and  $\langle c_F \rangle(y, t) = 0.9 \pm 0.005$  (trailing edge), respectively. Moreover, Figs. 6(a) and 6(b) show the conditioned fuel consumption and heat release rates, respectively, sampled from the leading edge. All these quantities sampled from the leading edges in cases D and D/O<sub>2</sub> are significantly larger than the counterpart quantities sampled from the

leading edges in cases D/T and D1 (basically similar results obtained from C, E, and F sets of flames, characterized by a lower  $Ka$  are not shown for brevity).

The huge difference between conditioned fuel consumption or heat release rates, reported in Fig. 6, can make the conditioned rates different after averaging over the entire flame brush. Such an interpretation is supported by the fact that the conditioned rates are higher in case D/O<sub>2</sub> than in case D in both Figs. 3 and 6, whereas  $\langle T^2 - \langle T|_{c_F} \rangle^2 |_{c_F} \rangle^{1/2}$  shows the opposite behavior in Fig. 4.

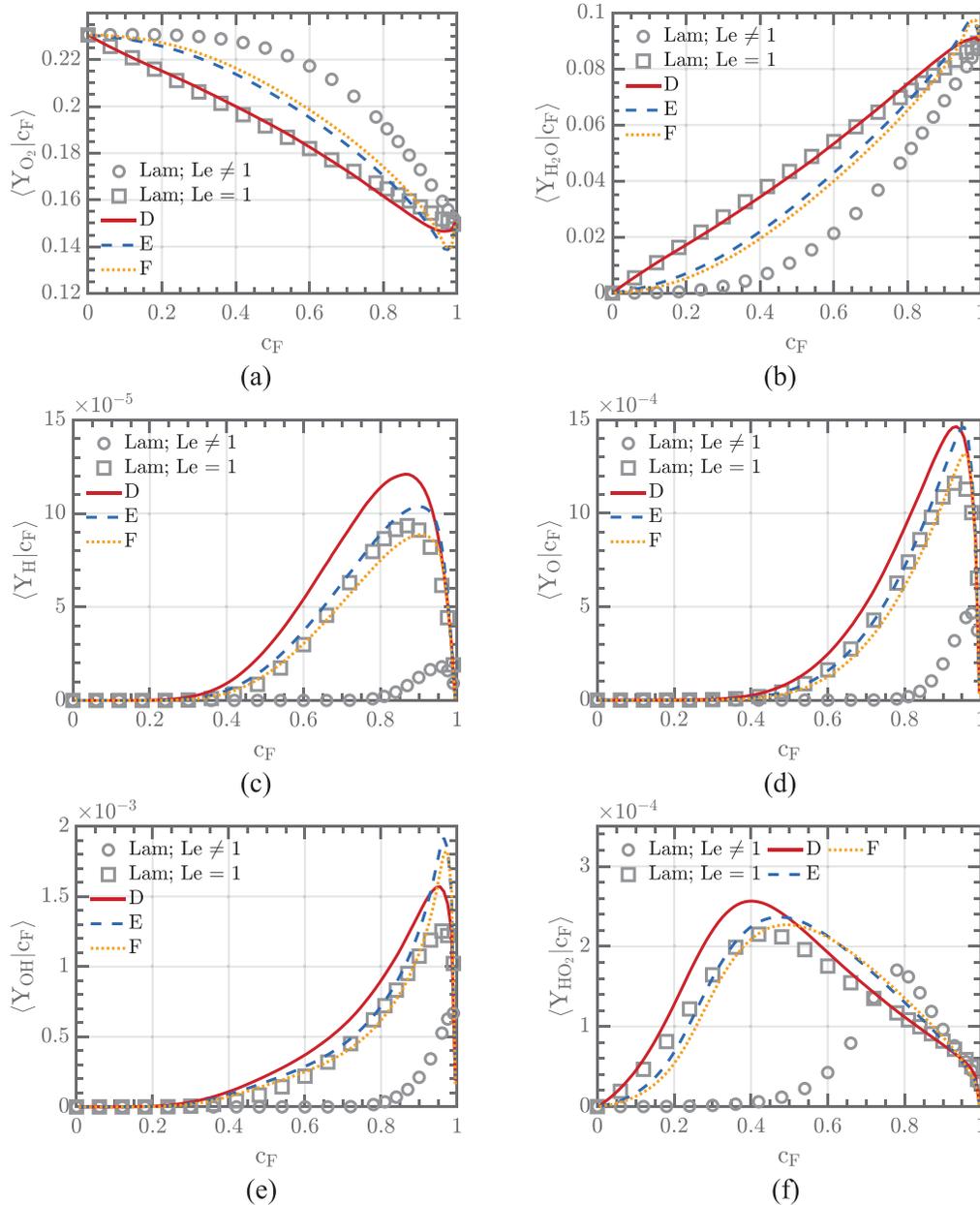


FIG. 7. Conditioned profiles of mass fractions of (a) O<sub>2</sub>, (b) H<sub>2</sub>O, (c) H, (d) O, (e) OH, and (f) HO<sub>2</sub>, extracted from entire flame brushes in cases D (red solid lines), E (blue dashed lines), and F (orange dotted lines). Circles and squares show  $Y_k(c_F)$  obtained from low Lewis number and equidiffusive laminar flames, respectively.

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The highlighted differences, documented at the flame leading edges, are mainly associated with the dominance of highly and positively (products in curvature center) curved reaction zones near flame leading edge, as discussed in detail for flame C elsewhere.<sup>31</sup> Briefly speaking, if  $Le$  is significantly less than unity, temperature is locally increased in highly and positively curved reaction zones, because the molecular flux of chemical energy (bond in a light fuel with a high diffusivity) into these reaction zones overwhelms the heat flux from these zones. Such effects are well explored for stretched laminar flames.<sup>20,22–26</sup>

All the results reported in Figs. 1–6 are consistent with each other if the turbulent burning velocity is controlled by processes localized to the flame leading edge, in line with the leading point concept. As reviewed elsewhere,<sup>13,20,26</sup> the concept was pioneered by the Russian school. Subsequently, it was adapted to predict abnormally high turbulent burning velocities measured in very lean hydrogen flames.<sup>41,42</sup> Over the past decade, the concept was supported by analyzing experimental<sup>14,16,17</sup> or DNS<sup>43–45</sup> data, including data obtained from the present flames C and C1,<sup>31</sup> as well as in theoretical studies<sup>46–48</sup> and in Reynolds-averaged Navier–Stokes simulations<sup>49</sup> of Atlanta experiments<sup>14,16</sup> with lean syngas–air turbulent flames. Not only are the present DNS data consistent with the leading point concept, but they also strongly support it.

Thus, on the one hand, Figs. 1, 5, and 6 show that Lewis number effects should be taken into account when modeling turbulent burning velocity. On the other hand, Fig. 2 implies that such effects could be neglected when evaluating the conditioned temperature at high  $Ka$ . Such a simplification is also supported in Fig. 7, which shows that the conditioned profiles of species mass fractions either (i) tend to profiles obtained from the equidiffusive laminar flame ( $O_2$  and  $H_2O$ ) when  $Ka$  is increased or (ii) are sufficiently close to the equidiffusive laminar flame profiles ( $H$ ,  $O$ ,  $OH$ , and  $HO_2$ ) at various  $Ka$ . This observation suggests that, even in lean  $H_2$ –air flames with pronounced Lewis number effects, the mean concentrations of various species in intense turbulence could be modeled by averaging a linear combination of the concentration profiles pre-computed for counterpart low Lewis number and equidiffusive laminar flames. The profile weights in such a linear combination could depend on  $Ka$  or/and another non-dimensional flame characteristic (e.g.,  $u'/S_L$ ,  $L/\delta_L^T$ , or  $Da$ ). A comparison of Figs. 7(a) and 7(b) with Figs. 7(c)–7(f) implies that these weights could be different for major reactants or products and for radicals. This issue deserves further study and will be addressed in future publications.

#### IV. CONCLUSIONS

A significant increase in turbulent burning velocity  $U_T^E$  (both dimensional and normalized with the laminar flame speed  $S_L$ ) due to differences in molecular transport coefficients is documented at a Karlovitz number  $Ka$  as high as 565.

The phenomenon is controlled by the Lewis number effects, whereas preferential diffusion plays a minor (if any) role.

This increase in  $U_T^E$  is more pronounced in leaner flames, with all other things being equal.

While the conditioned temperature profiles sampled from the entire flame brushes at high  $Ka$  are not sensitive to variations in molecular transport coefficients, similar profiles sampled from the

leading edges of the flame brushes show significant increase in the local temperature in the case of a low Lewis number. Such effects are even more pronounced for fuel consumption and heat release rates. These results are fully consistent with the computed increase in  $U_T^E$  due to Lewis number effects and further illuminate the crucial role played by processes localized to the leading edge of a turbulent flame brush in its propagation. Therefore, Lewis number effects should not be disregarded when evaluating the turbulent burning velocity even at high  $Ka$ .

On the contrary, the use of temperature and species mass fraction profiles pre-computed for equidiffusive laminar flames could work reasonably well when evaluating the mean temperature and species mass fractions provided that an advanced predictive model of the probability density function  $P(c_F)$  is available. Readers interested in recent progresses in modeling  $P(c_F)$  in premixed turbulent flames are referred to the latest publications.<sup>50–57</sup>

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#### AUTHOR DECLARATIONS

##### Conflict of Interest

The authors have no conflicts to disclose.

#### DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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