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# Effects of thermal expansion on moderately intense turbulence in premixed flames

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## Abstract

The study aims at analytically and numerically exploring the influence of combustion-induced thermal expansion on turbulence in premixed flames. In the theoretical part, contributions of solenoidal and potential velocity fluctuations to the unclosed component of the advection term in the Reynolds-averaged Navier-Stokes equations are compared and a new criterion for assessing the importance of the thermal expansion effects is introduced. The criterion highlights a ratio of the dilatation in the laminar flame to the large-scale gradient of root-mean-square (rms) velocity in the turbulent flame brush. To support the theoretical study, direct numerical simulation (DNS) data obtained earlier from two complex-chemistry, lean H<sub>2</sub>-air flames are analyzed. In line with the new criterion, even at sufficiently high Karlovitz numbers, results show significant influence of combustion-induced potential velocity fluctuations on the second moments of the turbulent velocity upstream of and within the flame brush. In particular, the DNS data demonstrate that (i) potential and solenoidal rms velocities are comparable in the unburnt gas close to the leading edge of the flame brush and (ii) potential and solenoidal rms velocities conditioned to unburnt gas are comparable within the entire flame brush. Moreover, combustion-induced thermal expansion affects not only the potential velocity, but even the solenoidal one. The latter effects manifest themselves in a negative correlation between solenoidal velocity fluctuations and dilatation or in the counter-gradient behavior of the solenoidal scalar flux. Finally, a turbulence-in-premixed-flame diagram is sketched to discuss the influence of combustion-induced thermal expansion on various ranges of turbulence spectrum.

## 32 I. INTRODUCTION

33 Since the pioneering work by Karlovitz et al.<sup>1</sup> and Libby and Bray,<sup>2</sup> effects of thermal  
34 expansion on turbulence (e.g., so-called flame-generated turbulence<sup>1</sup>) and turbulent scalar  
35 transport (e.g., so-called counter-gradient diffusion<sup>2</sup>) in premixed flames have long been a  
36 challenging research subject.<sup>3-15</sup> Numerical studies reviewed elsewhere<sup>16-19</sup> indicate that the  
37 influence of combustion-induced thermal expansion on turbulence within a premixed flame  
38 brush is well (hardly) pronounced in weakly (highly) turbulent flames. Recent Direct  
39 Numerical Simulation<sup>11,20-23</sup> (DNS) and experimental<sup>24,25</sup> investigations further support this  
40 view. However, criteria for finding domains of importance of such an influence have not yet  
41 been well established.

42 One of the widely accepted criteria of this kind was suggested by Bray<sup>26</sup> who considered  
43 turbulent scalar transport to be counter-gradient if

$$44 \quad N_B = \frac{(\sigma-1)S_L}{2\alpha u'} > 1. \quad (1)$$

45 Here,  $\sigma = \rho_u/\rho_b$  is the density ratio;  $S_L$  is the laminar flame speed;  $u'$  is root-mean-square  
46 (rms) turbulent velocity; subscript  $u$  or  $b$  designates unburnt or burnt mixture, respectively;  
47 and the number  $N_B$  is known as Bray number. The factor  $\alpha$  is of unity order and is expected  
48 to increase with increasing a ratio of an integral length scale  $L$  of turbulence to the laminar  
49 flame thickness  $\delta_L$ .<sup>27</sup> Since a widely accepted model of  $\alpha$  has not yet been developed, this  
50 factor is often omitted in Eq. (1). In any case, turbulent scalar transport is not the major subject  
51 of the present study, which is rather focused on the influence of combustion-induced thermal  
52 expansion on the second moments of the turbulent velocity field.

53 By considering the influence of combustion-induced thermal expansion on small-scale  
54 turbulent eddies, Bilger<sup>28</sup> has hypothesized that such an influence is significant if the  
55 magnitude  $\tau_K^{-1}$  of velocity gradients in the smallest eddies is less than dilation  $\Theta =$   
56  $(\sigma - 1)\tau_f^{-1}$  in the laminar flame. Therefore, the following criterion should hold

$$57 \quad Ka < Ka_{cr}^B = \sigma - 1 \quad (2)$$

58 in order for the influence of combustion-induced thermal expansion on small-scale turbulent  
59 eddies to be substantial. Here,  $Ka = \tau_f/\tau_K$  designates Karlovitz number;  $\tau_f = \delta_L/S_L$  and  
60  $\tau_K = \eta_K/u_K = (\nu_u/\bar{\epsilon})^{1/2}$  are the laminar flame and Kolmogorov time scales, respectively;  
61  $u_K = (\nu_u\bar{\epsilon})^{1/4}$  and  $\eta_K = (\nu_u^3/\bar{\epsilon})^{1/4}$  are Kolmogorov velocity and length scales<sup>25</sup>,  
62 respectively;  $\nu$  is the kinematic viscosity of unburnt mixture;  $\bar{\epsilon} = 2\nu\overline{S_{jk}S_{jk}}$  is a mean  
63 dissipation rate;  $S_{jk} = 0.5(\partial u_j/\partial x_k + \partial u_k/\partial x_j)$  is the rate-of-strain tensor; and summation  
64 convention applies to repeated indices. Note that (i) under conditions of a low Mach number,  
65 as in the case under study, dilatational contribution to the mean dissipation rate is commonly  
66 neglected if turbulence characteristics in  $Ka$  are evaluated in the incompressible flow of  
67 unburnt reactants; and (ii) to properly characterize the dilatation magnitude, the laminar flame  
68 thickness should be evaluated as follows:  $\delta_L = (T_b - T_u)/\max|\nabla T|$ , where  $T$  is the  
69 temperature. The simple criterion given by Eq. (2) was recently supported in a DNS study<sup>30,31</sup>  
70 of two stoichiometric H<sub>2</sub>-air jet turbulent flames characterized by  $Ka = 3.7 < Ka_{cr}^B = 6.7$   
71 and  $Ka = 54 > Ka_{cr}^B$ .

72 Besides the influence of combustion-induced thermal expansion on the smallest turbulent  
73 eddies, addressed by Bilger,<sup>28</sup> larger eddies from the inertial range of Kolmogorov  
74 turbulence<sup>29</sup> may also be affected by the thermal expansion in flames.<sup>10,32</sup> In particular,  
75 O'Brien et al.<sup>32</sup> have theorized that thermal energy released by combustion and transformed

76 to kinetic energy at small scales can be transferred via inverse turbulence cascade to larger  
 77 eddies (this phenomenon is known as backscatter) whose time scale is shorter than or equal  
 78 to  $\tau_f$ . MacArt and Mueller<sup>10</sup> have also argued that “competition between a heat-release-  
 79 induced cascade and the classical, production-driven forward cascade” can appear under  
 80 certain conditions even if  $Ka > Ka_{cr}^B$ .

81 As far as the largest turbulent eddies, whose length scale is on the order of  $L$ , are concerned,  
 82 the present authors are not aware of a criterion characterizing the influence of combustion-  
 83 induced thermal expansion on such eddies. This work aims primarily at bridging this  
 84 knowledge gap.

85 In Sect. II, a new criterion is introduced by analyzing contributions of potential and  
 86 solenoidal components of a fluctuating velocity field to various terms in transport equations  
 87 for turbulent Reynolds stresses. To support this theoretical analysis, such potential and  
 88 solenoidal contributions are explored by processing published DNS data described briefly in  
 89 Sect. III. Results are reported in Sect. IV. The newly proposed criterion is compared with  
 90 other relevant criteria in Sect. V, where a simple diagram is drawn to speculate what ranges  
 91 of turbulence spectrum are substantially affected by combustion-induced thermal expansion  
 92 in a premixed flame under various conditions. Conclusions are summarized in Sect. VI.

93 It is worth stressing that (i) the newly introduced criterion complements criteria suggested  
 94 earlier, e.g., Eq. (2), rather than replacing them and (ii) another effect of combustion on  
 95 turbulence, i.e., turbulence decay due to an increase in kinematic viscosity with the  
 96 temperature, is not explored in the present paper, while this mechanism is considered in the  
 97 DNS discussed in Sects. III and IV.

## 98 II. A THEORETICAL ANALYSIS

### 99 A. Reynolds-average framework

100 Let us consider the Reynolds-averaged Navier-Stokes equations written in a non-  
101 conservative form:

$$102 \quad \frac{\partial \bar{u}_i}{\partial t} + \bar{u}_k \frac{\partial \bar{u}_i}{\partial x_k} + \overline{u'_k \frac{\partial u'_i}{\partial x_k}} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \frac{1}{\rho} \frac{\partial \tau_{ik}}{\partial x_k}. \quad (3)$$

103 Here,  $u_i = \bar{u}_i + u'_i$  is  $i$ -th component of the velocity vector  $\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}'$ ;  $t$  designates time;  $x_i$   
104 are Cartesian coordinates;  $p$  is the pressure;  $\tau_{ik}$  is the viscous stress tensor; and overbars  
105 designate Reynolds averages.

106 For constant-density flows, turbulence models aim at closing the Reynolds stresses  $\overline{u'_i u'_k}$  or  
107 the last term on the left-hand side (LHS) of Eq. (3). Moreover, in constant-density turbulence  
108 in an unbounded domain,  $\mathbf{u}'(\mathbf{x}, t)$  stems from a solenoidal (rotational) motion and  $\nabla \cdot \mathbf{u}' = 0$ .  
109 In flames,  $\nabla \cdot \mathbf{u}' \neq 0$  due to thermal expansion, with combustion-induced pressure  
110 perturbations creating potential (irrotational) velocity fluctuations. Thus, eventual importance  
111 of combustion-induced thermal expansion effects could be assessed by comparing  
112 contributions of solenoidal and potential velocity fields to major turbulence characteristics. In  
113 the following, this task is pursued by examining the last term on the LHS of Eq. (3).

114 If one performs a Helmholtz-Hodge decomposition (HHD) of the velocity field  $\mathbf{u}'(\mathbf{x}, t)$  into  
115 divergence-free solenoidal and irrotational potential fields,  $\mathbf{u}'_s(\mathbf{x}, t)$  and  $\mathbf{u}'_p(\mathbf{x}, t)$ , respectively,  
116 the following equations hold<sup>33</sup>

$$117 \quad u'_i = u'_{s,i} + u'_{p,i}; \quad \frac{\partial u'_{s,k}}{\partial x_k} = 0; \quad \frac{\partial u'_{p,k}}{\partial x_i} = \frac{\partial u'_{p,i}}{\partial x_k}. \quad (4)$$

118 The last equality results directly from  $\nabla \times \mathbf{u}'_p = 0$ . Substitution of Eqs. (4) into the last term  
119 on the LHS of Eq. (3) yields

$$\begin{aligned} 120 \quad \overline{u'_k \frac{\partial u'_l}{\partial x_k}} &= \overline{u'_{s,k} \frac{\partial u'_{s,l}}{\partial x_k}} + \overline{u'_{s,k} \frac{\partial u'_{p,l}}{\partial x_k}} + \overline{u'_{p,k} \frac{\partial u'_{s,l}}{\partial x_k}} + \overline{u'_{p,k} \frac{\partial u'_{p,l}}{\partial x_k}} \\ 121 \quad &= \frac{\partial \overline{u'_{s,l} u'_{s,k}}}{\partial x_k} + \frac{\partial \overline{u'_{p,l} u'_{s,k}}}{\partial x_k} + \frac{\partial \overline{u'_{p,k} u'_{s,l}}}{\partial x_k} - \overline{u'_{s,l} \frac{\partial u'_{p,k}}{\partial x_k}} + \overline{u'_{p,k} \frac{\partial u'_{p,l}}{\partial x_l}} \\ 122 \quad &= \frac{\partial}{\partial x_k} (\overline{u'_{s,l} u'_{s,k}} + \overline{u'_{p,l} u'_{s,k}} + \overline{u'_{s,l} u'_{p,k}}) + \frac{1}{2} \frac{\partial}{\partial x_l} \overline{u'_{p,k} u'_{p,k}} - \overline{u'_{s,l} \frac{\partial u'_{p,k}}{\partial x_k}}. \end{aligned} \quad (5)$$

123 The last term in the second line of Eq. (5) results from substitution of the last equality in Eq.  
124 (4) into the last term in the first line of Eq. (5).

125 In the simplest statistically one-dimensional (1D) and planar case, Eq. (5) reads

$$126 \quad \overline{u'_k \frac{\partial u'_l}{\partial x_k}} = \underbrace{\frac{\partial \overline{u'^2_{s,1}}}{\partial x_1}}_{T_1} + 2 \underbrace{\frac{\partial \overline{u'_{s,1} u'_{p,1}}}{\partial x_1}}_{T_2} + \underbrace{\frac{1}{2} \frac{\partial \overline{u'^2_{p,k} u'_{p,k}}}{\partial x_1}}_{T_3} - \underbrace{u'_{s,1} \frac{\partial u'_{p,k}}{\partial x_k}}_{T_4}. \quad (6)$$

127 Close to a boundary of importance of the studied thermal expansion effects, the order of  
128 magnitude of the potential velocity fluctuations cannot be larger than the order of magnitude  
129 of the rotational velocity fluctuations. Accordingly, within the mean flame brush, the order of  
130 magnitude of the first three terms on the right hand (RHS) of Eq. (6) is  $u'^2/\delta_t$  or less. Here,  
131  $\delta_t$  is the mean flame brush thickness.

132 To estimate the order of magnitude of the last term, let us, first, similarly to Bilger,<sup>28</sup> assume  
133 that  $|\nabla \cdot \mathbf{u}'_p|$  is on the order of  $\Theta = (\sigma - 1)\tau_f^{-1}$ . This assumption is in line with recent DNS  
134 and experimental data, which indicate that combustion is mainly localized to inherently  
135 laminar flamelets even at sufficiently high  $Ka$ , as reviewed elsewhere.<sup>34,35</sup> DNS data reported  
136 in Sect. IV support this assumption. It is also worth remembering that eventual decrease in

dilatation due to local flame broadening by small-scale turbulent eddies may be counterbalanced by (i) an increase in the dilatation magnitude due to straining of the local flame by larger turbulent eddies<sup>36</sup> and (ii) differential diffusion effects,<sup>37</sup> which are discussed in detail elsewhere.<sup>38</sup>

Second, to estimate the magnitude of the fourth term, let us also note that the correlation between solenoidal velocity fluctuations  $\mathbf{u}'_s$  and dilatation  $\nabla \cdot \mathbf{u}'_p$  does not vanish, because the vorticity transport equation involves a dilatation term.<sup>16-19</sup> This consideration will also be supported in Sect. IV.

Thus, the fourth term on the RHS of Eq. (6) is expected to be on the order of  $u'\theta = u'(\sigma - 1)\tau_f^{-1}$  bearing in mind that  $\mathbf{u}'_s$  and  $\mathbf{u}'$  are of the same order when the thermal expansion effects become relatively weak (close to the boundary we seek for). Therefore, the considered term, which involves potential velocity fluctuations, should play an important role unless the dilatation  $\theta$  is much smaller than  $u'/\delta_t$ . Contrary to Eq. (2), this newly introduced criterion compares  $\theta$  with the large-scale gradient of the rms turbulent velocity in the mean flame brush, rather than with the small-scale velocity gradient in Kolmogorov eddies. As the former gradient is significantly smaller, the newly introduced criterion implies importance of thermal expansion effects in a wider domain of flame characteristics.

According to the new criterion, thermal expansion effects are of minor importance if the Damköhler number  $Da = \tau_t/\tau_f$  is less than a critical value of

$$Da_{cr}^{-1} = (\sigma - 1) \frac{\delta_t}{L}, \quad (7)$$

where  $\tau_t = L/u'$  is an integral time scale of turbulence.

The same criterion can be obtained in a different way. Let us consider the following well-known Reynolds-averaged transport equation<sup>16-19,26,35</sup>

$$\frac{\partial c}{\partial t} + u_k \frac{\partial c}{\partial x_k} = \frac{1}{\rho} \frac{\partial q_{c,k}}{\partial x_k} + \frac{1}{\rho} \dot{\omega}_c \quad (8)$$

for a combustion progress variable  $c$ , which characterizes mixture state in a flame and varies from zero in unburnt reactants to unity in the equilibrium adiabatic combustion products. Here,  $q_{c,k}$  is  $k$ -th component of molecular flux  $\mathbf{q}_c$  of  $c$  and  $\dot{\omega}_c$  is the mass rate of product creation. The convection term, i.e., the second term on the LHS of Eq. (8), reads

$$u_k \frac{\partial c}{\partial x_k} = \frac{\partial u_k c}{\partial x_k} - c \frac{\partial u_k}{\partial x_k} = \frac{\partial u_{s,k} c}{\partial x_k} + \frac{\partial u_{p,k} c}{\partial x_k} - c \frac{\partial u_{p,k}}{\partial x_k}. \quad (9)$$

For the reasons presented above, within the mean flame brush, the order of magnitude of the first two terms on the RHS of Eq. (9) is  $u'/\delta_t$  or less, whereas the order of magnitude of the third term is  $\Theta$ . Thus, we arrive at Eq. (7) again.

In Eq. (7), the thickness  $\delta_t$  is unknown *a priori*. Various experimental<sup>39-42</sup> and DNS<sup>34,43-45</sup> data show that  $\delta_t/L > 1$ . Therefore,  $Da_{cr}$  should be less than  $(\sigma - 1)^{-1} = O(10^{-1})$ . Moreover, DNS data<sup>43,44</sup> indicate that mean thickness of a fully-developed turbulent premixed flame, i.e., a turbulent premixed flame propagating at a constant speed and having a constant thickness, scales as  $\delta_{t,\infty}/L \propto (u'/S_L)^{1/3}$  in moderately intense ( $u'/S_L \leq 10$ ,  $Da > 0.2$ ) turbulence, whereas a subsequent DNS study<sup>34</sup> has yielded  $\delta_{t,\infty}/L \propto Da^{-1/2}$  at  $Da < 0.1$ . Here, the subscript  $\infty$  refers to the fully-developed flame. Let us invoke the latter scaling for  $\delta_t/L$ , because Eq. (7) implies that a small  $Da < O(10^{-1})$  is required for the thermal expansion effects to be of minor importance in turbulent flames. We arrive at

$$Da_{cr} = (\sigma - 1)^{-2} \quad (10)$$

by disregarding numerical factors of unity order.

In the following the thickness  $\delta_t = (T_b - T_u)/\max|\nabla \bar{T}|$  will be extracted from the DNS data.

## 182 B. Favre-average framework

183 In the combustion literature, Favre averaging is often used to reduce the number of unclosed  
184 terms in the Favre-averaged transport equations when compared to the Reynolds-averaged  
185 ones. Therefore, it is worth comparing contributions of potential and solenoidal velocities to  
186 the Favre-averaged second moments  $\overline{\rho u_i'' u_k''}$ . Here,  $u_i'' \equiv u_i - \tilde{u}_i$  and  $\tilde{u}_i \equiv \overline{\rho u_i} / \bar{\rho}$ . However,  
187 defining Favre-averaged fluctuating solenoidal and potential velocity fields is not trivial.  
188 Indeed, because

$$\begin{aligned} 189 \quad u_i'' &= u_i - \tilde{u}_i = \bar{u}_i + u_i' - \tilde{u}_i = \bar{u}_i + u_i' - \frac{\overline{\rho u_i}}{\bar{\rho}} \\ 190 \quad &= \bar{u}_i + u_i' - \frac{\overline{\rho u_i}}{\bar{\rho}} - \frac{\overline{\rho u_i'}}{\bar{\rho}} = u_i' - \frac{\overline{\rho u_i'}}{\bar{\rho}} = u_i' - \tilde{u}_i', \end{aligned} \quad (11)$$

191 the fields  $\mathbf{u}'(\mathbf{x}, t)$  and  $\mathbf{u}''(\mathbf{x}, t)$  cannot be divergence-free (or irrotational) simultaneously.  
192 Since  $\mathbf{u}'(\mathbf{x}, t)$  directly characterizes the fluctuating velocity field, whereas  $\mathbf{u}''(\mathbf{x}, t)$  is also  
193 affected by the density, HHD should be applied to  $\mathbf{u}'(\mathbf{x}, t)$ , followed by computation of the  
194 velocities  $\mathbf{u}_s''$  and  $\mathbf{u}_p''$  using Eq. (11), i.e.,

$$195 \quad u_{s,i}'' \equiv u_{s,i}' - \tilde{u}_{s,i}', \quad u_{p,i}'' \equiv u_{p,i}' - \tilde{u}_{p,i}'. \quad (12)$$

196 Subsequently, contributions of the solenoidal and potential velocity fields to the Favre-  
197 averaged Reynolds stress term can be evaluated as follows

$$198 \quad \frac{\partial}{\partial x_k} \overline{\rho u_i'' u_k''} = \underbrace{\frac{\partial}{\partial x_k} \overline{\rho u_{s,i}'' u_{s,k}''}}_{T_1} + \underbrace{\frac{\partial}{\partial x_k} \overline{\rho u_{p,i}'' u_{p,k}''}}_{T_2} + \underbrace{\frac{\partial}{\partial x_k} \overline{\rho u_{p,i}'' u_{s,k}''} + \frac{\partial}{\partial x_k} \overline{\rho u_{s,i}'' u_{p,k}''}}_{T_3}, \quad (13)$$

199 where  $u_{s,i}''$  and  $u_{p,i}''$  are defined by Eq. (12). Various terms in Eqs. (6) and (13) will be  
200 compared in Sect. IV by analyzing DNS data obtained from two flames characterized by  
201 different  $Ka$ .

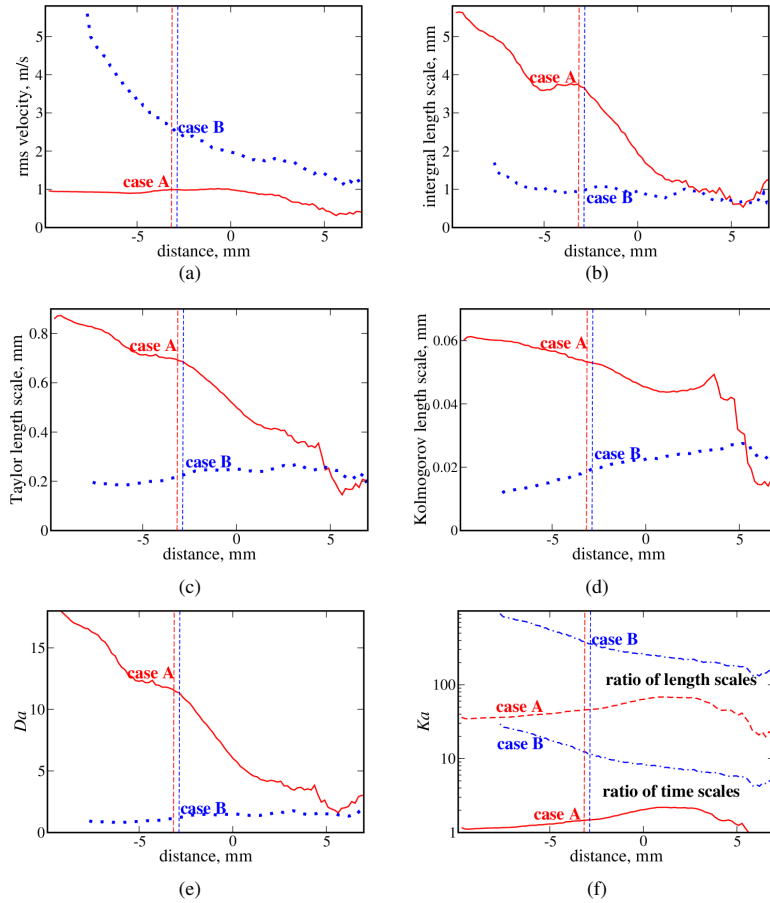
202 Note that the Favre-averaged convection term is also affected by fluctuating solenoidal and  
 203 potential velocities. Indeed, substitution of  $\tilde{u}_i = \overline{u_i} + \tilde{u}'_i = \bar{u}_i + \tilde{u}'_i$  into a product of  $\tilde{u}_i \tilde{u}_k$ ,  
 204 followed by application of HHD to the fields  $\bar{\mathbf{u}}(\mathbf{x}, t)$  and  $\mathbf{u}'(\mathbf{x}, t)$  results in a sum of 16 terms.  
 205 In the statistically 1D and planar case,  $\bar{u}_{p,1} = \bar{u}_1$ ,  $\bar{u}_{s,1} = 0$ , and

$$\begin{aligned} \frac{\partial}{\partial x_1} (\bar{\rho} \tilde{u}_1^2) = & \underbrace{\frac{\partial}{\partial x_1} (\bar{\rho} \tilde{u}_{s,1} \tilde{u}_{s,1})}_{\tilde{T}_1} + 2 \underbrace{\frac{\partial}{\partial x_1} (\bar{\rho} \tilde{u}_{s,1} \bar{u}_1)}_{\tilde{T}_2} + 2 \underbrace{\frac{\partial}{\partial x_1} (\bar{\rho} \tilde{u}_{s,1} \tilde{u}_{p,1})}_{\tilde{T}_3} \\ & + \underbrace{\frac{\partial}{\partial x_1} (\bar{\rho} \bar{u}_1^2)}_{\tilde{T}_4} + 2 \underbrace{\frac{\partial}{\partial x_1} (\bar{\rho} \tilde{u}_{p,1} \bar{u}_1)}_{\tilde{T}_5} + \underbrace{\frac{\partial}{\partial x_1} (\bar{\rho} \tilde{u}_{p,1} \tilde{u}_{p,1})}_{\tilde{T}_6}. \end{aligned} \quad (14)$$

### 208 III. NUMERICAL SIMULATIONS

#### 209 A. DNS conditions

210 As the DNS attributes and data were reported earlier,<sup>11,15,46-48</sup> only a brief description is  
 211 given below, with more details being reported in Appendix A. Unconfined statistically 1D  
 212 and planar, lean (the equivalence ratio  $\Phi=0.7$ )  $\text{H}_2$ -air turbulent flames were investigated by (i)  
 213 adopting a detailed (9 species, 23 reversible reactions) chemical mechanism<sup>49</sup> with the  
 214 mixture-averaged transport model and (ii) numerically solving unsteady three-dimensional  
 215 governing equations, written in compressible form. Note that while differential diffusion  
 216 effects are well known to be highly pronounced in very lean  $\text{H}_2$ -air flames and to significantly  
 217 increase turbulent burning velocity, as reviewed elsewhere,<sup>38</sup> differential diffusion was  
 218 shown<sup>50,51</sup> to weakly affect a mean bulk burning rate at  $\Phi=0.7$ . For this reason, the equivalence  
 219 ratio was set equal to 0.7 in the present study.



**FIG. 1.** Axial variations of turbulent flame characteristics conditioned to unburned mixture in flames A (red lines) and B (blue lines). Vertical dotted-dashed lines show the flame-brush leading edge, i.e., planes characterized by  $\bar{c}(\xi) = 0.05$ . (a) rms turbulent velocity  $u'$ , (b) integral length scale  $L_{KE}$ , (c) Taylor microscale  $\lambda$ , (d) Kolmogorov length scale  $\eta_K$ , (e) Damköhler number, (f) Karlovitz number  $Ka = \tau_f/\tau_K$  and  $(\delta_L/\eta_K)^2$ .

Two cases A and B, characterized by two different values of the inlet rms velocity, with all other things being equal, were studied. Variations of the major turbulence characteristics along the  $x$ -axis in these two cases are shown in Fig. 1. Here, the distance  $\xi$  is counted from a transverse plane characterized by  $\langle c \rangle(x, t) = 0.5$  at each instant, i.e.,  $\langle c \rangle(\xi, t) = 0.5$ ; the

225 combustion progress variable  $c$  is defined using fuel mass fraction; all reported quantities  
 226  $\langle \cdot | c < 0.02 \rangle$  are conditioned to unburned mixture, i.e., to  $c(\mathbf{x}, t) < 0.02$ , and, subsequently,  
 227 are transverse and time-averaged;  $u' = \sqrt{2\langle u'_k u'_k | c < 0.02 \rangle / 3}$ ;  $L_{k\varepsilon} =$   
 228  $\langle 0.5 u'_k u'_k | c < 0.02 \rangle^{3/2} / \langle \varepsilon | c < 0.02 \rangle$ ;  $Da = L_{k\varepsilon} S_L / (u' \delta_L)$ ;  $Ka = \tau_f / \tau_K$ , with a ratio of  
 229  $(\delta_L / \eta_K)^2$  being also plotted in Fig. 1f;  $\tau_K = (\nu_u / \langle \varepsilon | c < 0.02 \rangle)^{1/2}$  and  $\eta_K =$   
 230  $(\nu_u^3 / \langle \varepsilon | c < 0.02 \rangle)^{1/4}$ ;  $\lambda = 15 \nu_u u'^2 / \langle \varepsilon | c < 0.02 \rangle$  is Taylor microscale; and the local  
 231 dissipation rate  $\varepsilon = 2 \nu_u S_{jk} S_{jk}$ . A slow decrease in  $\eta_K$  with the streamwise distance near the  
 232 leading edge of flame A (see red solid line in Fig. 1d) is attributed to the influence of  
 233 combustion-induced thermal expansion on turbulence upstream of the flame, as will be  
 234 discussed later (see Fig. 7a in Sect. IV).

235

	Table I. Relevant parameters characterizing the DNS cases.								
	$u'_0/S_L$	$L_T/\delta_L$	$Re_T$	$u'/S_L$	$L_{k\varepsilon}/\delta_L$	$Da$	$Ka$	$(\delta_L/\eta_K)^2$	$Da_{cr}$
A	0.7	14	227	0.7	10.3	11	1.5	46	0.11
B	5.0	14	1623	1.9	2.7	1.2	12	385	0.03

236 Major characteristics of the injected turbulence and major turbulent flame characteristics  
 237 evaluated at the leading edges of the two flame brushes are reported in Table I. Here,  $u'_0$  is the  
 238 rms velocity in the injected flow;  $L_T$  is the most energetic length scale of the Passot-Pouquet  
 239 spectrum;<sup>52</sup>  $Re_T = u'_0 L_T / \nu_u$ ; the quantities  $u'$ ,  $L_{k\varepsilon}$ ,  $Da$ , and  $Ka$  have been sampled at  $\overline{c(\xi)} =$   
 240 0.05;  $S_L = 1.36$  m/s,  $\delta_L = 0.36$  mm,  $\sigma = 6.7$ , and, hence,  $Ka_{cr}^B = 5.7$  have been computed  
 241 under the simulation conditions (atmospheric pressure and  $T_u = 300$  K);  $Da_{cr}$  has been  
 242 calculated using Eq. (7) and the DNS data on  $\delta_t = (T_b - T_u) / \max|\nabla \bar{T}|$ , whereas Eq. (10)  
 243 yields  $Da_{cr} = 0.03$  for both flames. In case B, Eqs. (7) and (10) yield close results. In case  
 244 A, the Damköhler number is significantly higher; consequently, scaling of  $\delta_t \propto \delta_L \sqrt{Re_T}$  does  
 245 not hold and results yielded by Eqs. (7) and (10) are different. Note also that  $(\delta_L/\eta_K)^2$  is

much larger than  $Ka = \tau_f / \tau_K$ , because  $\delta_L = (T_b - T_u) / \max|\nabla T| \gg \nu_u / S_L$  in the studied complex-chemistry case.

The criteria introduced in Sect. II, both Eq. (7) and Eq. (10), imply that combustion-induced thermal expansion can substantially affect the large-scale turbulence characteristics in both flames A and B. On the contrary, Eq. (2) suggests that the influence of the thermal expansion on the small-scale turbulence characteristics can be of importance in flame A only, whereas  $Ka > Ka_{cr}^B$  in case B.

When processing the DNS data, transverse-averaged quantities  $\langle \cdot \rangle(\xi, t)$  were sampled first, followed by time-averaging of them. Time and transverse-averaged quantities are designated with overbar, e.g.,  $\bar{c}(\xi) \equiv \overline{\langle c \rangle(\xi, t)}$ .

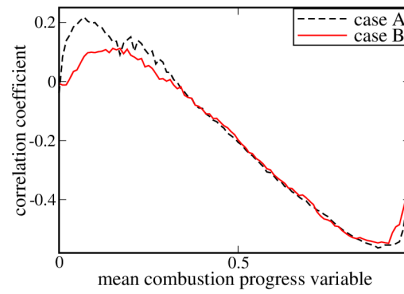
#### B. Helmholtz-Hodge decomposition

The fluctuating velocity  $\mathbf{u}'(\mathbf{x}, t)$  was decomposed into solenoidal and potential components  $\mathbf{u}'_s(\mathbf{x}, t)$  and  $\mathbf{u}'_p(\mathbf{x}, t)$  by using two methods: (i) conventional<sup>33</sup> HHD and (ii) natural<sup>53,54</sup> decompositions. To do so, algorithms that were applied earlier by the present authors to velocity fields obtained from weakly turbulent single-step chemistry flames<sup>55,56</sup> and from flames<sup>15</sup> A and B were adopted. The reader interested in a detailed discussion of these algorithms is referred to the latter paper.<sup>15</sup> Since the earlier results yielded by the two decompositions were hardly distinguishable within flame brushes,<sup>55</sup> we will report results obtained using the former method only.

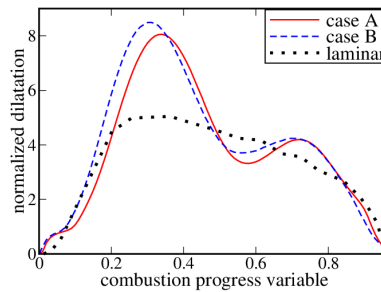
The fields  $\mathbf{u}''_s(\mathbf{x}, t)$  and  $\mathbf{u}''_p(\mathbf{x}, t)$  were computed using Eq. (12). Note that  $\nabla \cdot \mathbf{u}''_s \neq 0$  and  $\nabla \times \mathbf{u}''_p \neq 0$ .

#### IV. NUMERICAL RESULTS AND DISCUSSION

To obtain Eqs. (7) and (10) in Sect. II, two assumptions were invoked: (i) correlation between solenoidal velocity fluctuations and dilatation did not vanish and (ii) the order of magnitude of local dilatation in turbulent premixed flames could be estimated using the laminar-flame value  $\Theta$ . These assumptions are validated in Figs. 2 and 3, respectively.



**FIG. 2.** Correlation coefficient  $\overline{u'_{s,1} \nabla \cdot \mathbf{u}'_p} / [\overline{u'^2_{s,1}} (\nabla \cdot \mathbf{u}'_p)^2]^{1/2}$  vs. mean combustion progress  $\bar{c}$ .



**FIG. 3.** Conditioned dilatation  $\langle \nabla \cdot \mathbf{u} | c \rangle$  sampled from the entire computational domain in case A or B, as well as dependence of  $\nabla \cdot \mathbf{u}$  on  $c$  in the counterpart laminar flame.

More specifically, Fig. 3 shows that the conditioned dilatation  $\langle \nabla \cdot \mathbf{u} | c \rangle$  is indeed on the order of  $\nabla \cdot \mathbf{u}(c)$  in the laminar flame, while the former can be larger than the latter. A similar quantitative difference was reported in earlier DNS studies.<sup>36,37</sup> Such a difference can be

280 controlled by three physical mechanisms: (i) local flame thinning due to turbulent stretch rates,  
 281 (ii) local flame broadening due to small-scale turbulent mixing, and (iii) differential diffusion  
 282 effects if molecular transport coefficients for fuel, oxidant, and heat are substantially different.  
 283 Mechanisms (i) and (ii) always compete and can either decrease or increase the local flame  
 284 thickness depending on conditions.<sup>57</sup> Accordingly, the local dilatation is either increased or  
 285 decreased, respectively. Differential diffusion effects can change not only the local flame  
 286 thickness but also the local normal velocity jump at the flame. While for the considered  
 287 mixture, mean bulk burning rate was shown to be weakly affected by differential diffusion,  
 288 variations in the local flame characteristics were also documented.<sup>50,51</sup> Further discussion of  
 289 Fig. 3 is beyond the scope of the present work, and differences between the turbulent  $\langle \nabla \cdot \mathbf{u} | c \rangle$ ,  
 290 see solid and dashed lines, and the laminar  $\nabla \cdot \mathbf{u}(c)$ , see dotted line, could be addressed in a  
 291 future study.

292 Figure 4 shows variations of all terms in Eq. (6) within mean flame brushes. Note that the  
 293 almost perfect agreement between the LHS and RHS of this equation in both cases, cf. black  
 294 solid and brown dotted lines, verifies conservation in the simulations. Contrary to the criterion  
 295 given by Eq. (2), but in line with the newly introduced criterion given by Eq. (7), thermal  
 296 expansion effects are well pronounced not only in flame A, but also in flame B. More  
 297 specifically, the magnitude of the last term ( $T_4$ ), which contains dilatation and, hence, arises  
 298 due to thermal expansion, is comparable with or larger than the magnitude of the purely  
 299 solenoidal term  $T_1$ . Furthermore, at  $\bar{c} > 0.5$ , the former term dominates within both flames,  
 300 i.e.,  $|T_4|$  is much larger than  $|T_1 + T_2 + T_3|$ . These DNS data clearly show importance of  
 301 thermal expansion effects under conditions of the present study, thus, supporting the analysis  
 302 in Sect. II. Note that (i)  $T_4 < 0$  at  $\bar{c} > 0.5$  because dilatation reduces vorticity in flames,<sup>16-19</sup>  
 303 i.e., correlation between solenoidal velocity fluctuations and dilatation is predominantly

negative (see Fig. 2); but (ii) the RHS of Eq. (6) is positive because it includes  $T_4$  with a minus sign.

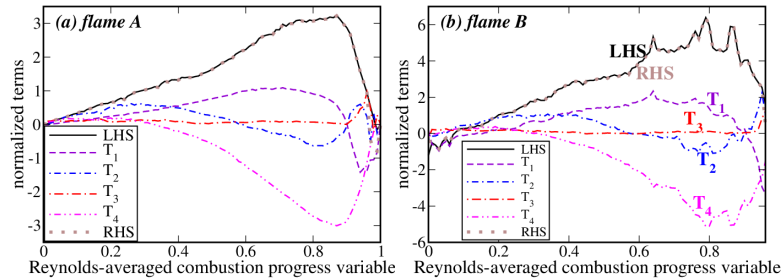


FIG. 4. Various terms in Eq. (6), normalized using  $S_L$  and  $\delta_L$ , in flames (a) A and (b) B.

Importance of thermal expansion effects is also shown in Fig. 5, which reports various terms in Eq. (13) for the two statistically one-dimensional planar flames (note almost perfect matching between the LHS and RHS again). Although the magnitude of the solenoidal term  $T_1$  is larger than the magnitudes of other terms at  $\bar{c} > 0.5$  in both flames and at  $\bar{c} < 0.2$  in flame B, term  $T_3$ , which involves both solenoidal and potential velocities, also plays an important role. Even the potential term  $T_2$  is not negligible.

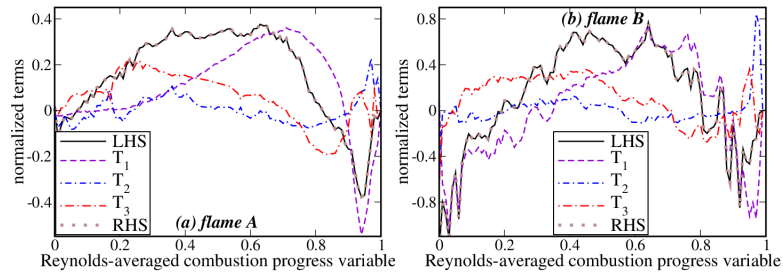
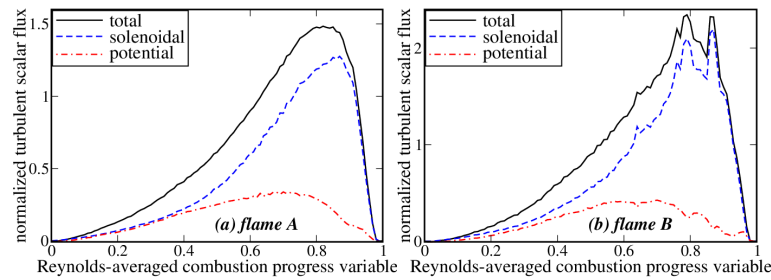


FIG. 5. Various terms in Eq. (13), normalized using  $\rho_u$ ,  $S_L$ , and  $\delta_L$ , in flames (a) A and (b) B.

At the same time, comparison of Figs. 4 and 5 indicates that thermal expansion effects are less pronounced within the Favre-averaging framework, i.e., the dilatation term ( $T_4$ )

dominates at  $\bar{c} > 0.5$  on the RHS of Eq. (6), whereas the solenoidal term ( $T_1$ ) is the most important term on the RHS of Eq. (13) in the largest parts of the two flame brushes. However, this result does not mean that the use of Favre-averaged velocities is favorable in solving the problem of modeling turbulence in flames. The fact that the solenoidal term is the largest term on the RHS of Eq. (13) at  $\bar{c} > 0.5$  does not prove that models developed for solenoidal incompressible turbulent flows hold for the solenoidal term on the RHS of Eq. (13) in flames. Rather, combustion-induced thermal expansion can substantially affect not only potential velocity fluctuations, but also solenoidal turbulence even at high  $Ka$ . Two examples follow.

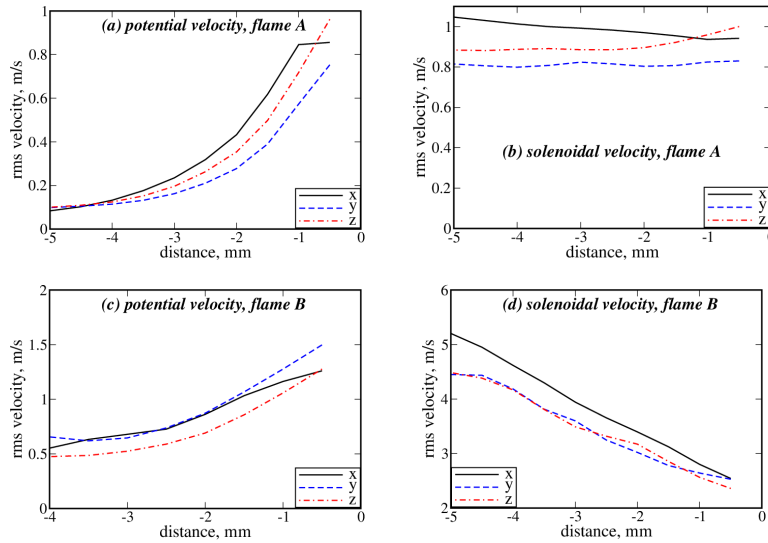
First, Fig. 3 and a large magnitude of term  $T_4$  on the RHS of Eq. (6) (see Fig. 4) show a well-pronounced negative (at  $\bar{c} > 0.4$ ) correlation between dilatation and solenoidal velocity fluctuations, thus implying a substantial influence of thermal expansion on the solenoidal velocity field in the studied flames.



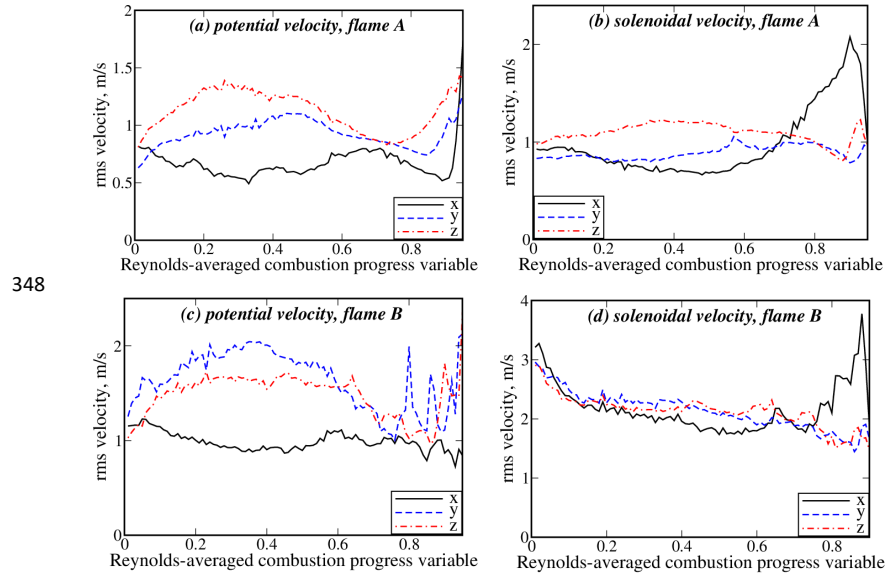
**FIG. 6.** Axial turbulent scalar flux normalized using  $\rho_u$  and  $S_L$  in flames (a) A and (b) B.

Second, Fig. 6 shows that not only the total turbulent scalar flux  $\overline{\rho u'' c''}$ , but also its solenoidal and potential components are counter-gradient ( $d\bar{c}/dx > 0$  in the studied flames). The counter-gradient behavior of  $\overline{\rho u_s'' c''}$  indicates a substantial influence of thermal expansion on the solenoidal velocity in the considered flames. This influence is attributed to vorticity that is generated by baroclinic torque. As discussed in detail elsewhere,<sup>6,8</sup> such a

337 vorticity acts to push the leading and trailing segments of the instantaneous flame inside the  
 338 mean flame brush. Thus, for a flame propagating from right to left, fluctuations in the local  
 339  $u_s$ , caused by baroclinic torque, are positive and negative at  $\bar{c} \ll 1$  and  $1 - \bar{c} \ll 1$ ,  
 340 respectively. Fluctuations in the local  $c$ , caused by appearance of the instantaneous flame, are  
 341 also positive and negative in these zones, respectively. Therefore,  $u'_s$  correlates positively with  
 342  $c'$ . It is worth noting that the obtained counter-gradient behavior of the flux  $\overline{\rho u'' c''}$  does not  
 343 contradict the well-known Bray number criterion,<sup>26,27</sup> because  $u'/S_L < \sigma - 1$  even in case B.  
 344 As evidenced by the above analysis, there is substantial influence of combustion-induced  
 345 thermal expansion not only on the total and potential velocity fluctuations, but also on the  
 346 solenoidal velocity fluctuations at  $Ka = \tau_f/\tau_K$  as large as 12 and  $(\delta_L/\eta_K)^2$  about 400.



**FIG. 7.** Variations of (a), (c) potential and (b), (d) solenoidal rms velocities  $(\overline{u_{lp}^2})^{1/2}$  and  $(\overline{u_{ls}^2})^{1/2}$ , respectively, upstream of flames (a)-(b) A and (c)-(d) B. Zero distance corresponds to  $\langle c \rangle(x, t) = 0.01$ .



**FIG. 8.** Variations of (a), (c) potential and (b), (d) solenoidal rms velocities conditioned to unburned mixture, i.e.,  $\langle u_{i,p}^2 | c(\mathbf{x}, t) < 0.01 \rangle^{1/2}$  and  $\langle u_{i,s}^2 | c(\mathbf{x}, t) < 0.01 \rangle^{1/2}$ , respectively, within flames (a)-(b) A and (c)-(d) B.

Further insights into the influence of combustion-induced thermal expansion on turbulence in flames can be obtained from Figs. 7 and 8. In particular, Figs. 7a and 7c show that the rms magnitude  $\langle u_{i,p}^2 \rangle^{1/2}$  of the potential velocity fluctuations increases upstream of the flame brush as the flow approaches the flame leading edge  $\langle c \rangle(x, t) = 0.01$ . This effect is attributed to generation of potential velocity fluctuations by combustion-induced pressure perturbations that propagate upstream of the flame. A similar physical mechanism is well known to cause the hydrodynamic instability of laminar premixed flames.<sup>58,59</sup> On the contrary, the solenoidal  $\langle u_{i,s}^2 \rangle^{1/2}$  decreases with distance from the inlet due to turbulence decay, which is much more pronounced in the highly turbulent case B. As a result, the potential and solenoidal rms

358 velocities are comparable in the region close to the flame leading edge, cf. rightmost points  
359 on curves in Figs. 7a and 7b for case A, and Figs. 7c and 7d for case B.

360 Last, Fig. 8 shows that rms values of potential and solenoidal velocity fluctuations,  
361 conditioned to unburned gas are comparable with one another within A or B-flame brush.

### 362 V. TURBULENCE-IN-PREMIXED-FLAME DIAGRAM

363 The goal of this section is to discuss different criteria of importance of thermal expansion  
364 effects in premixed flames and to present such criteria in a regime diagram. While this diagram  
365 seems similar to the classical premixed-turbulent-combustion regime-diagrams,<sup>60-62</sup> there is  
366 an important difference: the classical diagrams address the influence of turbulence on a  
367 premixed flame, whereas the present diagram considers the influence of a premixed flame on  
368 turbulence.

369 First, let us compare the two criteria given by Eqs. (2) and (10). Using the well-known  
370 scaling of  $Da^2 Ka^2 \propto Re_t = u'L/\nu$ , where constants of unity order are omitted for brevity,  
371 the critical number  $Da_{cr}$  could be substituted with  $\sqrt{Re_t}/Ka_{cr}$ . Accordingly, Eq. (10) reads

$$372 \quad Ka_{cr} = (\sigma - 1)^2 \sqrt{Re_t} = Ka_{cr}^B (\sigma - 1) \sqrt{Re_t} \gg Ka_{cr}^B. \quad (15)$$

373 Alternatively, Eq. (2) can be rewritten as follows

$$374 \quad Da_{cr}^B = \sqrt{Re_t} (\sigma - 1)^{-1} = (\sigma - 1) \sqrt{Re_t} Da_{cr} \gg Da_{cr}. \quad (16)$$

375 Thus, the newly introduced criterion substantially extends the domain of the influence of  
376 combustion-induced thermal expansion on turbulence in premixed flames to a higher  
377 Karlovitz number and a lower Damköhler number. The DNS data analyzed in Sect. IV and,  
378 in particular, Figs. 4, 5, 7, and 8 are consistent with this extension.

379 Second, as noted in Sect. I, O'Brien et al.<sup>28</sup> have theorized that backscatter can arise from  
 380 smaller scales, associated with injection of kinetic energy due to combustion, to larger scales  
 381 whose lifetime  $\tau_m$  is shorter than or equal to the laminar flame time scale  $\tau_f$ . In the inertial  
 382 range<sup>29</sup> of Kolmogorov turbulence, a constraint of  $\tau_m \leq \tau_f$  reads  $(l_m^2/\varepsilon)^{1/3} \leq \tau_f$  or

$$383 \quad l_m \leq (\bar{\varepsilon}\tau_f^3)^{1/2} = S_L^{-3/2}\delta_L^{3/2}(\nu_u/\tau_K^2)^{1/2} = \delta_L Ka\Gamma^{-1/2}, \quad (17)$$

384 with the length scale  $(\bar{\varepsilon}\tau_f^3)^{1/2}$  being earlier introduced by Corrsin.<sup>63</sup> Here, the number  $\Gamma \equiv$   
 385  $S_L\delta_L/\nu_u$ , known as “flame Reynolds number”, is larger than unity and can be as large as 50  
 386 in lean hydrogen-air mixtures under room conditions.<sup>64</sup> If the energy flux due to combustion  
 387 is localized to scales on the order of  $\delta_L$ ,<sup>65-67</sup> the scale  $l_m$  should be larger than  $\delta_L$ . Therefore,  
 388 Eq. (17) implies that backscatter could arise if  $Ka\Gamma^{-1/2} > 1$  or

$$389 \quad Ka > \Gamma^{1/2}. \quad (18)$$

390 If  $Ka < \Gamma^{1/2}$ , even the smallest turbulent eddies evolve slowly, such that combustion-induced  
 391 local velocity perturbations are associated with rapid distortion within the flame, and “any  
 392 cascade interaction through convective transport between small and large scales is relegated  
 393 to the far wake of the burnt gases.”<sup>32</sup>

394 Equation (17) is a necessary condition for existence of a spectral interval where backscatter  
 395 can be induced by combustion. However, to cause backscatter, combustion should be  
 396 sufficiently strong. By extending Bilgers' arguments,<sup>28</sup> let us hypothesize that backscatter may  
 397 arise if the dilatation  $\Theta$  is larger than the magnitude of turbulence-induced velocity gradient  
 398  $(\delta_L^2/\varepsilon)^{-1/3}$  at the scale  $l = \delta_L$ , associated with the energy injection due to combustion. Here,  
 399 this length scale is assumed to belong to the inertial range of turbulence spectrum, which  
 400 seems to be plausible if  $Ka > Ka_{cr}^B > 1$  (especially for lean hydrogen-air mixtures, where

401  $\delta_L/\eta_K \gg Ka^{1/2}$  under room conditions). Therefore, backscatter may arise in the inertial  
402 range if

$$403 \quad \Theta(\delta_L^2/\bar{\epsilon})^{1/3} = (\sigma - 1)S_L\delta_L^{-1/3}(\tau_K^2/\nu_u)^{1/3} = (\sigma - 1)Ka^{-2/3}(S_L\delta_L/\nu_u)^{1/3} > 1 \quad (19)$$

404 or

$$405 \quad Ka < Ka_{cr}^* = (\sigma - 1)^{3/2}\Gamma^{1/2} = (\sigma - 1)^{1/2}\Gamma^{1/2}Ka_{cr}^B. \quad (20)$$

406 Since  $Ka_{cr}^* > Ka_{cr}^B$  and  $\Gamma^{1/2} < Ka_{cr}^B$  for most fuels (or  $\Gamma^{1/2} \cong Ka_{cr}^B$  in lean hydrogen-air  
407 mixtures), Eqs. (18) and (20) are consistent with one another. Under conditions of  $\Gamma^{1/2} <$   
408  $Ka < Ka_{cr}^*$ , both  $\Gamma^{1/2} < Ka < Ka_{cr}^B$  and  $\Gamma^{1/2} < Ka_{cr}^B < Ka$  are possible, i.e., Eq. (2) may  
409 or may not hold. Thus, backscatter may arise even if the smallest-scale turbulent eddies are  
410 weakly affected by combustion-induced thermal expansion.

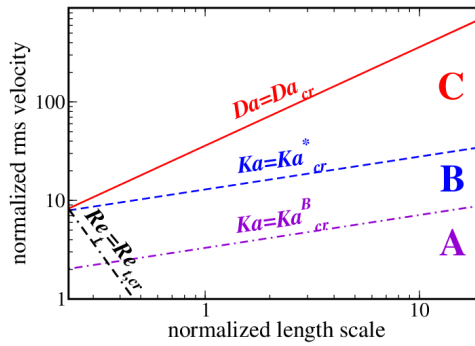
411 For the present flame B,  $Ka = 12$  (see Table I) is larger than  $Ka_{cr}^B = 5.7$ , but is smaller  
412 than  $Ka_{cr}^* = 75$ . Accordingly, substantial influence of combustion-induced thermal  
413 expansion on turbulent eddies from the inertial range is expected. Indeed, two-point second-  
414 order structure functions for the potential velocity field, which (i) were sampled from flame  
415 B, (ii) were conditioned to unburnt mixture, and (iii) were reported in a recent paper,<sup>15</sup> do  
416 show such an influence even at small distances  $r$  between two points where velocity is picked.  
417 In flame A characterized by  $Ka < Ka_{cr}^B$ , the effect is observed even at very small  $r$ , cf. Figs.  
418 4b and 4e or 4c and 4f in the cited paper, where flames A and B are labeled with letters W and  
419 H, respectively.

420 Using a scaling of  $Da^2Ka^2 \propto Re_t$ , Eq. (20) reads

$$421 \quad Da > Da_{cr}^* = \sqrt{Re_t}(\sigma - 1)^{-3/4}\Gamma^{-1/4} = \sqrt{Re_t}(\sigma - 1)^{5/4}\Gamma^{-1/4}Da_{cr}. \quad (21)$$

Therefore,  $Da_{cr}^* > Da_{cr}$  if  $Re_t > (\sigma - 1)^{-5/2} \Gamma^{1/2}$ , which holds in a turbulent flow, where  $Re_t \gg 1$ . Thus, when compared to Eq. (20), which allows for backscatter in the inertial range, the newly introduced criterion given by Eq. (10) substantially extends the domain of the influence of combustion-induced thermal expansion on turbulence in premixed flames to a lower Damköhler number.

In addition to the three criteria given by Eqs. (2), (10), and (20), one more criterion is worth mentioning. Hydrodynamic instability of laminar premixed flames<sup>58,59</sup> stems from velocity perturbations upstream of the flame, caused by combustion-induced pressure waves. Thus, the instability is an example of the discussed thermal expansion effects. However, as shown elsewhere,<sup>38,68-70</sup> the instability plays a minor role in premixed turbulent combustion if  $Ka$  is of unity order or larger. Therefore, the instability cannot change the three criteria given by Eqs. (2), (10), and (20).



**FIG. 9.** Turbulence-in-premixed-flame diagram  $\{L/\delta_L, u'/S_L\}$  sketched using Eq. (2) (violet dotted-dashed line), Eq. (10) (red solid line), Eq. (20) (blue dashed line), and Eq. (22) (black double-dashed-dotted line).  $\sigma = 7$ ,  $\Gamma = 10$ , and  $u'/S_L = Ka^{2/3}(L/\delta_L)^{1/3}$ . A: region of the influence of thermal expansion on small-scale turbulence. B: active cascade region. C: region of the influence of thermal expansion on large-scale turbulence.

The three criteria given by Eqs. (2), (10), and (20) are plotted in violet dotted-dashed, red solid, and blue dashed lines, respectively, in Fig. 9. To do so, values of  $\sigma = 7$  and  $\Gamma = 10$ ,

437 associated with near-stoichiometric methane-air mixtures under room conditions, were set and  
 438 the following simplified relation  $u'/S_L = Ka^{2/3}(L/\delta_L)^{1/3}$  was invoked. Since Eq. (10) was  
 439 obtained using Eq. (7) and the following scaling  $\delta_{t,\infty}/L \propto Re_t^{1/2}$ , extrapolation of Eq. (10) to  
 440 low length scale ratios  $L/\delta_L$  is limited by a constraint of  $\delta_{t,\infty} > \delta_L$  or

$$441 \quad Re_t > Re_{t,cr} = \left(\frac{\delta_L}{L}\right)^2. \quad (22)$$

442 In Fig. 9, this constraint is plotted in black double-dashed-dotted line.

443 In the domain bounded by Eqs. (10) and (20), combustion-induced thermal expansion can  
 444 affect large-scale turbulence characteristics, as discussed in Sects. III and V. In a band  
 445 bounded by Eqs. (2) and (20), the combustion-induced thermal expansion can also cause  
 446 backscatter in the inertial range of turbulence spectrum. Following O'Brien et al.,<sup>32</sup> this layer  
 447 is labeled “active cascade”. Note that Eq. (18) holds for the selected values of  $\sigma = 7$  and  $\Gamma =$   
 448 10. Finally, below the violet dotted-dashed line yielded by Eq. (2), the combustion-induced  
 449 thermal expansion can also affect the smallest turbulent eddies.

## 450 VI. CONCLUSIONS

451 A new criterion was introduced for assessing importance of turbulence modulations due to  
 452 combustion-induced thermal expansion in premixed flames. The criterion highlights a ratio of  
 453 dilatation in the laminar flame to the large-scale gradient of rms turbulent velocity across the  
 454 turbulent flame brush. When compared to the well-known Bilger's criterion,<sup>28</sup> the developed  
 455 criterion substantially expands domain of conditions associated with importance of thermal  
 456 expansion. It is worth stressing, however, that the present study extends Bilger's analysis,<sup>28</sup>  
 457 rather than contradicting it. The point is that Bilger<sup>28</sup> addressed the influence of combustion-

458 induced thermal expansion on small-scale turbulence characteristics, whereas the present  
459 work allows for large-scale effects.

460 Assumptions invoked to arrive to the newly introduced criterion were validated by  
461 analyzing DNS data obtained earlier from two complex-chemistry, lean H<sub>2</sub>-air flames  
462 propagating in a box. In line with the new criterion, results show significant influence of  
463 combustion-induced potential velocity fluctuations on evolution of the second moments of the  
464 turbulent velocity field upstream of and within both flame brushes. In particular, the DNS data  
465 show that (i) potential and solenoidal rms velocities are comparable in unburnt gas close to  
466 the leading edge of flame brush in each case and (ii) potential and solenoidal rms velocities  
467 conditioned to unburnt gas are comparable within entire flame brush in each case.

468 Moreover, the DNS data indicate that combustion-induced thermal expansion affects not  
469 only total and potential velocities, but also solenoidal velocity. Such effects manifest  
470 themselves in a negative correlation between the solenoidal velocity fluctuations and  
471 dilatation or in the counter-gradient behavior of the solenoidal scalar flux  $\overline{\rho u_s'' c''}$ . Therefore,  
472 the applicability of constant-density turbulence models to the solenoidal velocity fluctuations  
473 in flames may be subjected to scrutiny even at  $(\delta_L/\eta_K)^2$  about 400.

474 To summarize results of earlier relevant studies<sup>10,28,32</sup> and the present one, various regimes  
475 of the influence of combustion-induced thermal expansion on turbulence spectrum in  
476 premixed flames are outlined in a newly introduced turbulence-in-premixed-flame (TiPF)  
477 diagram.

#### 478 Declaration of Competing Interest

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

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490 **DATA AVAILABILITY**

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

493 **APPENDIX A: DNS ATTRIBUTES**

494 Simulations were performed in a rectangular domain of size of  $20 \times 10 \times 10 \text{ mm}^3$  using a  
495 uniform Cartesian mesh of  $512 \times 256 \times 256$  cells. The mesh ensured about ten grid points per  
496  $\delta_L$ , with Kolmogorov length scale being larger than cell size  $\Delta x$ . Unsteady three-dimensional  
497 partially differential transport equations were discretized using an eighth-order central  
498 difference scheme for internal mesh points, with the order of differentiation being gradually  
499 decreased to a one-sided fourth-order scheme near the inlet and outlet boundaries.<sup>71</sup> Time  
500 integration was performed adopting an explicit fourth-order Runge-Kutta scheme.<sup>71</sup>

Along the flame propagation direction, inflow and outflow characteristic boundary conditions were set using an improved Navier-Stokes characteristic boundary condition technique.<sup>72</sup> Other boundary conditions were periodic.

A divergence-free, isotropic, homogeneous turbulent velocity field was generated using a pseudo spectral method<sup>73</sup> and adopting the Passot-Pouquet spectrum.<sup>52</sup> The field was injected through the inlet (left) boundary and decayed along the mean flow direction ( $x$ -axis). At  $t = 0$ , a pre-computed planar laminar flame structure was embedded into the computational domain to initialize turbulent flame propagation from right to left along  $x$ -axis. Subsequently, the mean inlet flow velocity was gradually changed to match turbulent flame speed. Results reported in the present paper were sampled at six different instants in each case, i.e., at  $t/t_e = 0.57, 0.67, 0.77, 0.86, 0.96$ , and  $1.05$  in case A and at  $t/t_e = 4.1, 4.8, 5.5, 6.2, 6.8$ , and  $7.5$  in case B, where,  $t_e$  is the eddy turnover time.

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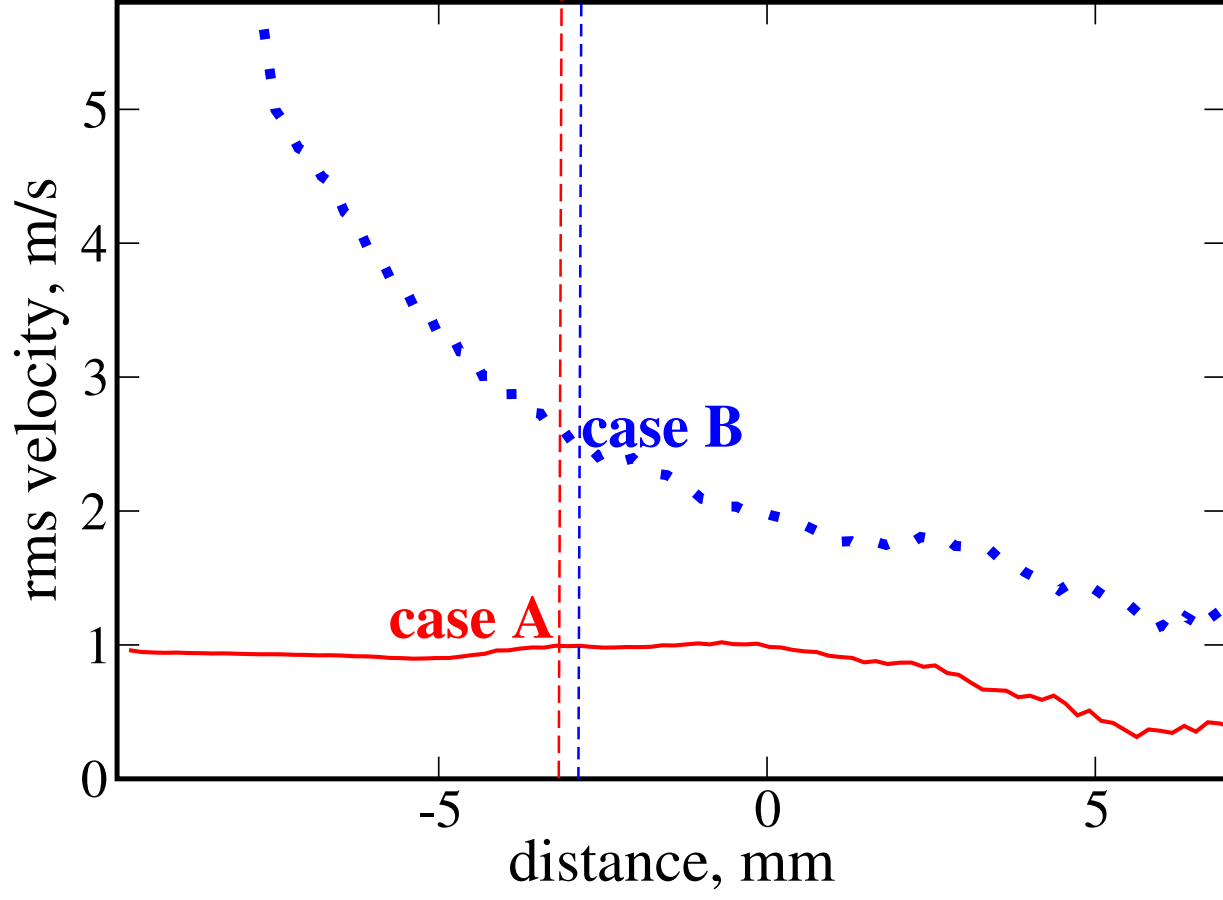
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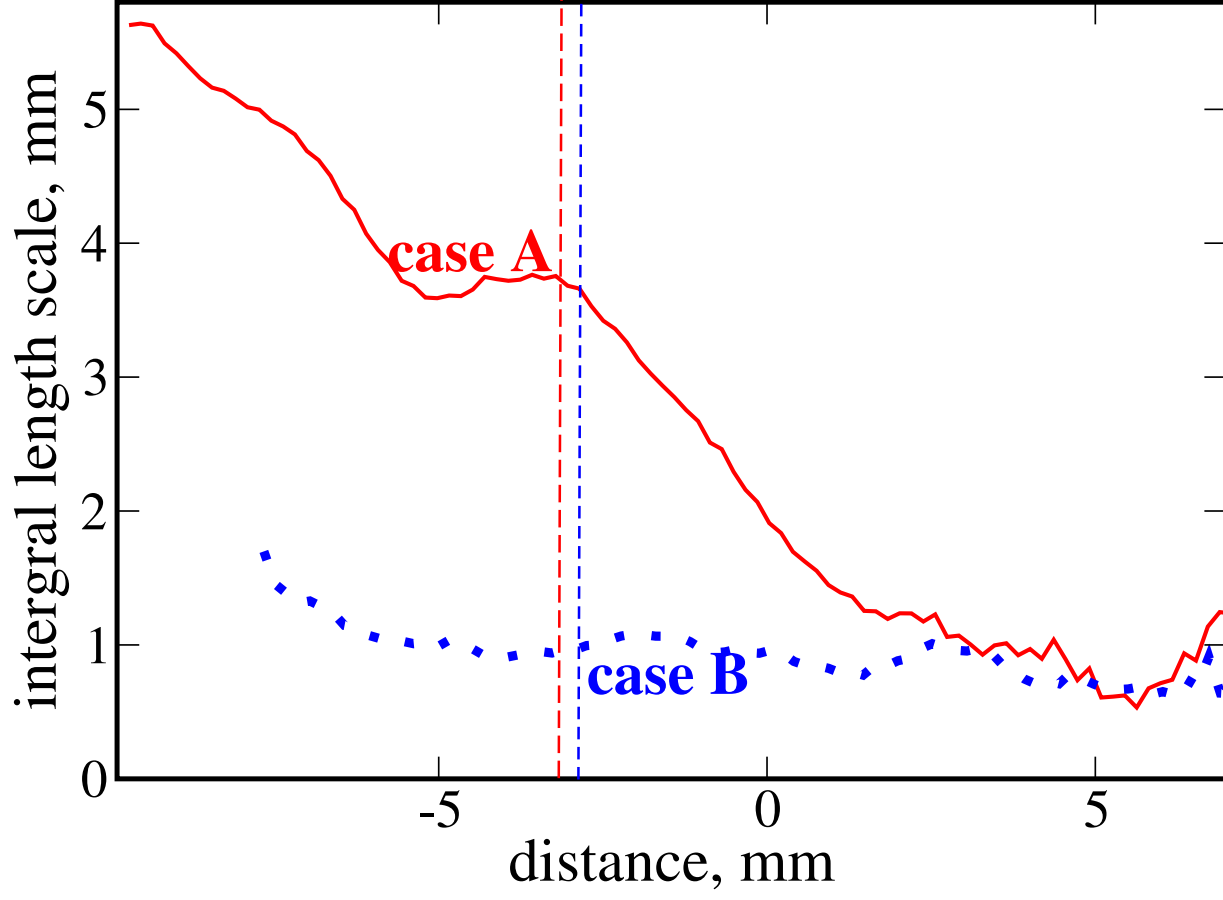
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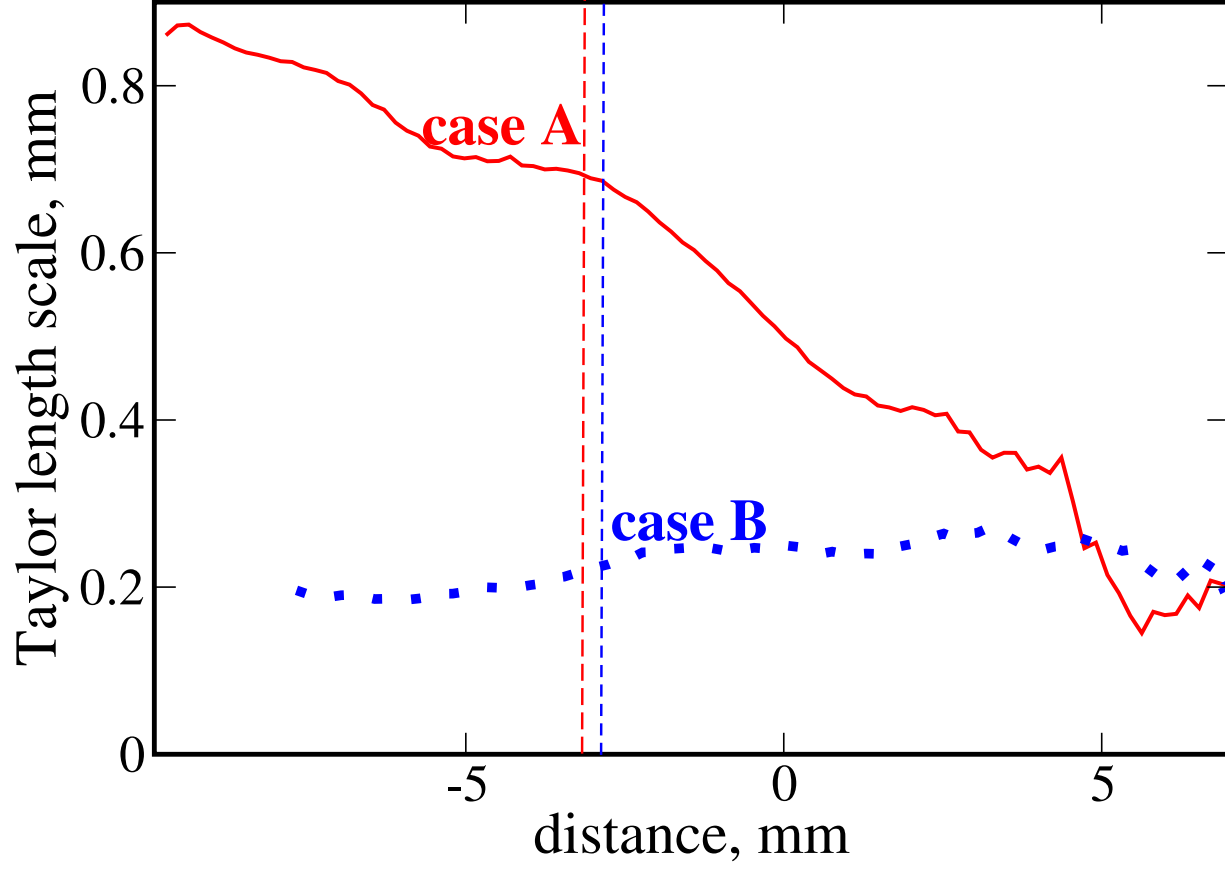
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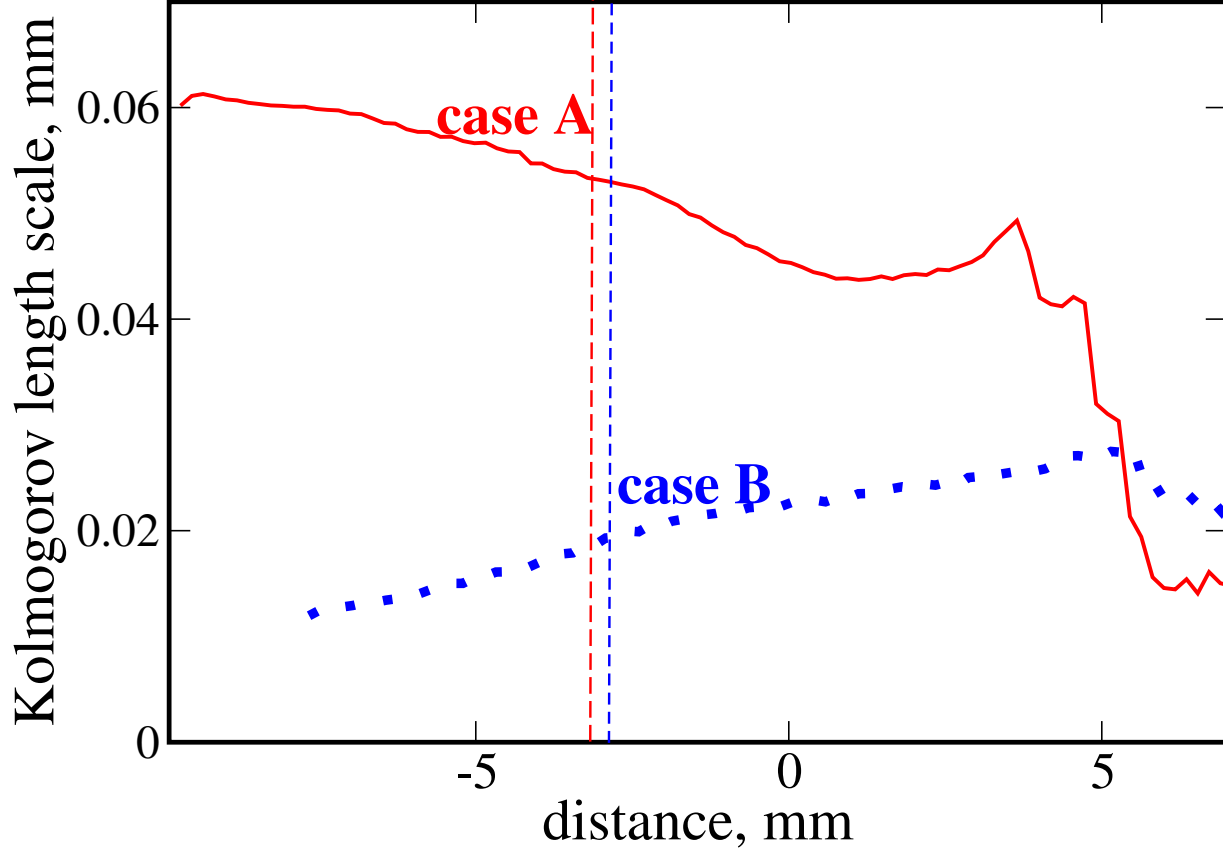
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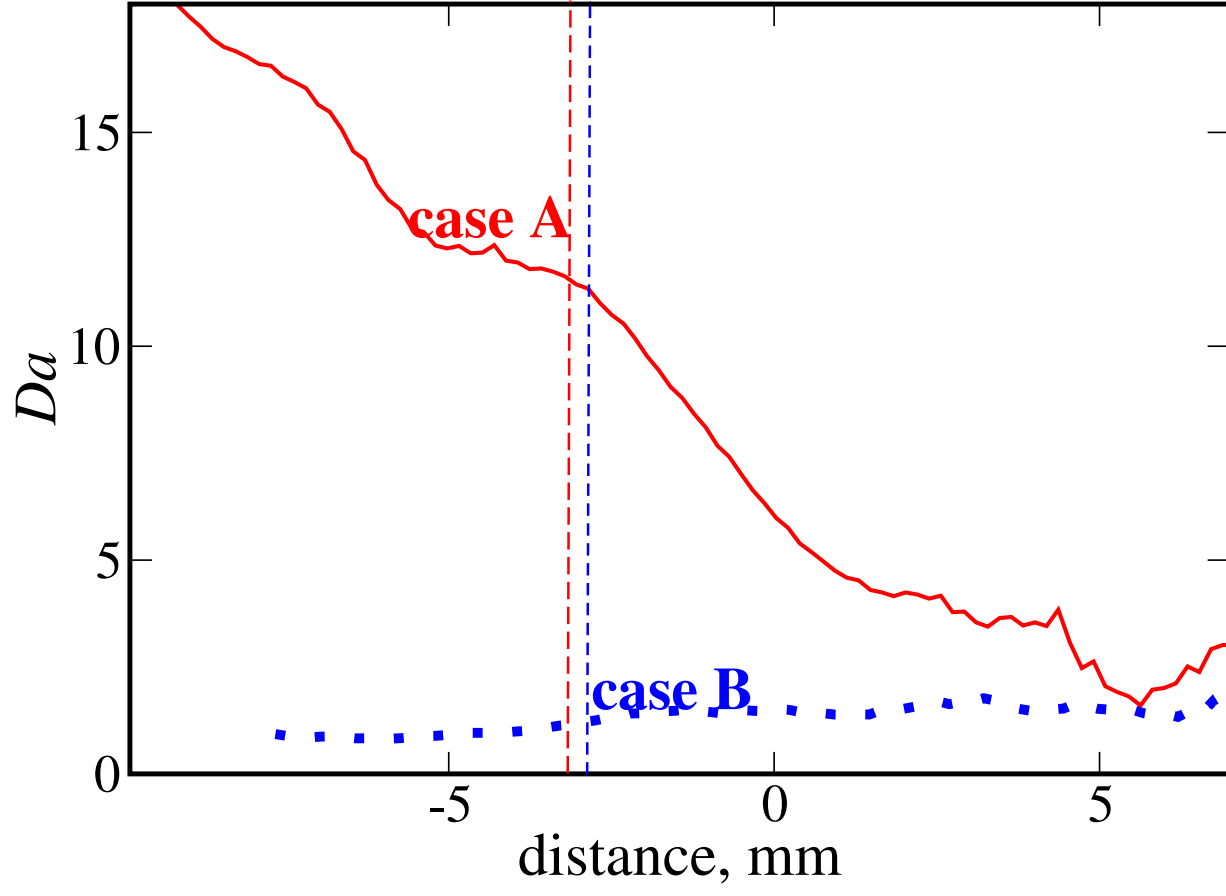
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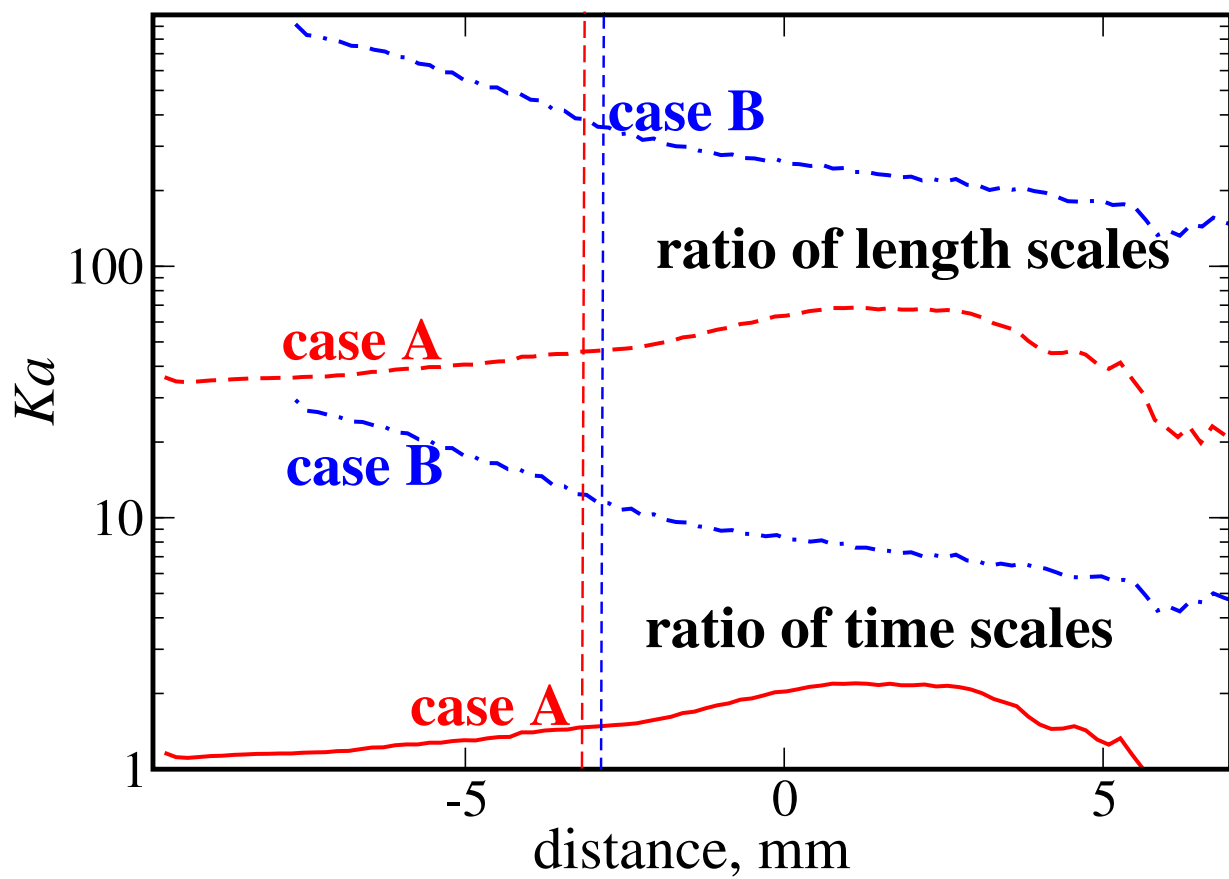
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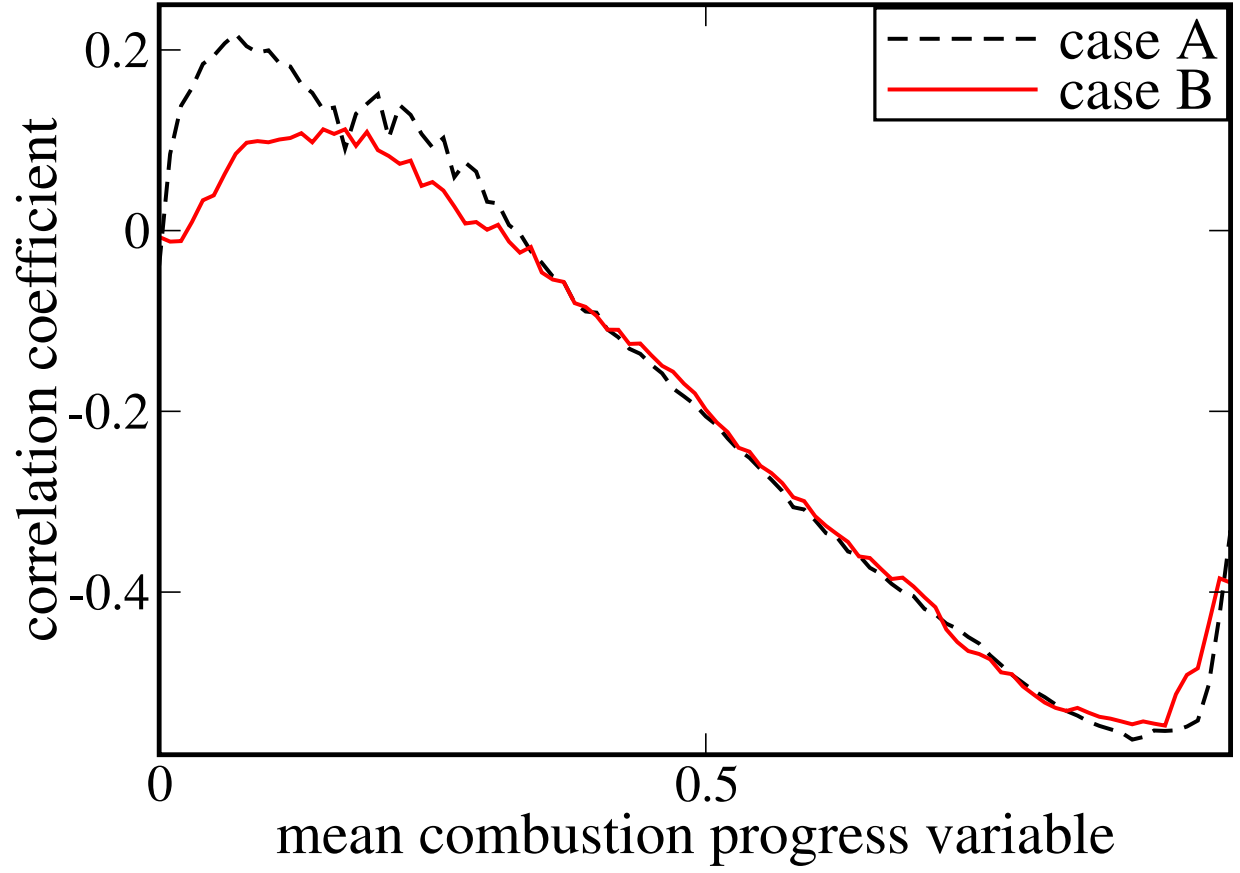
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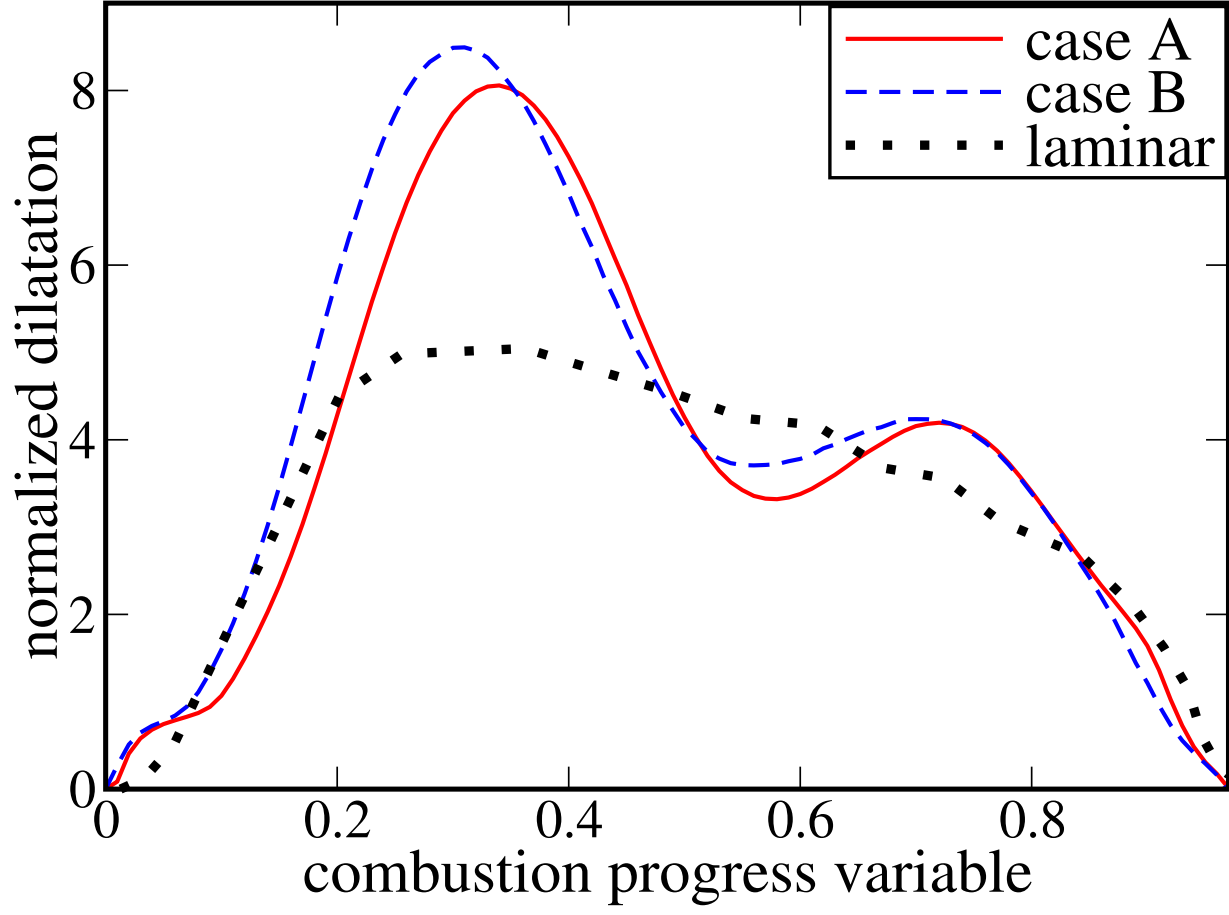
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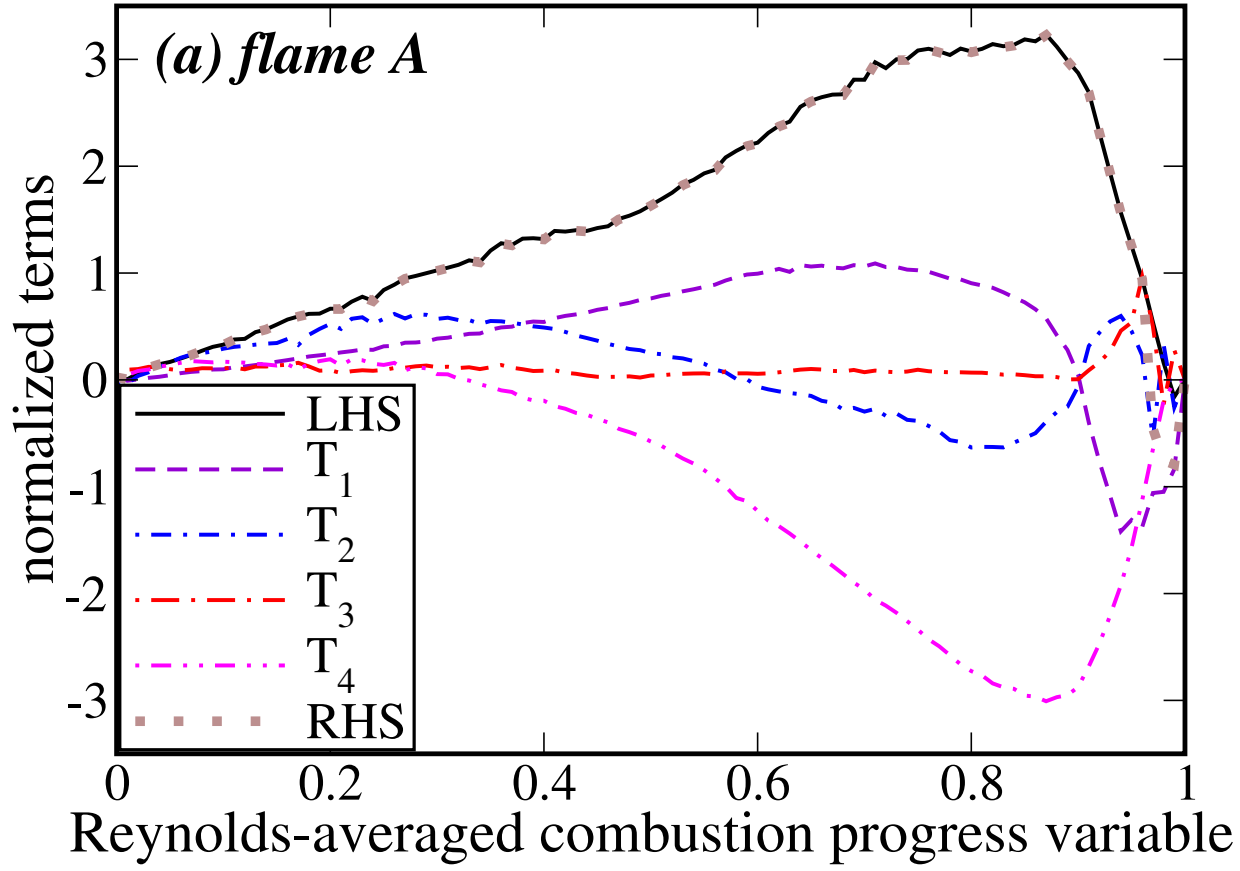
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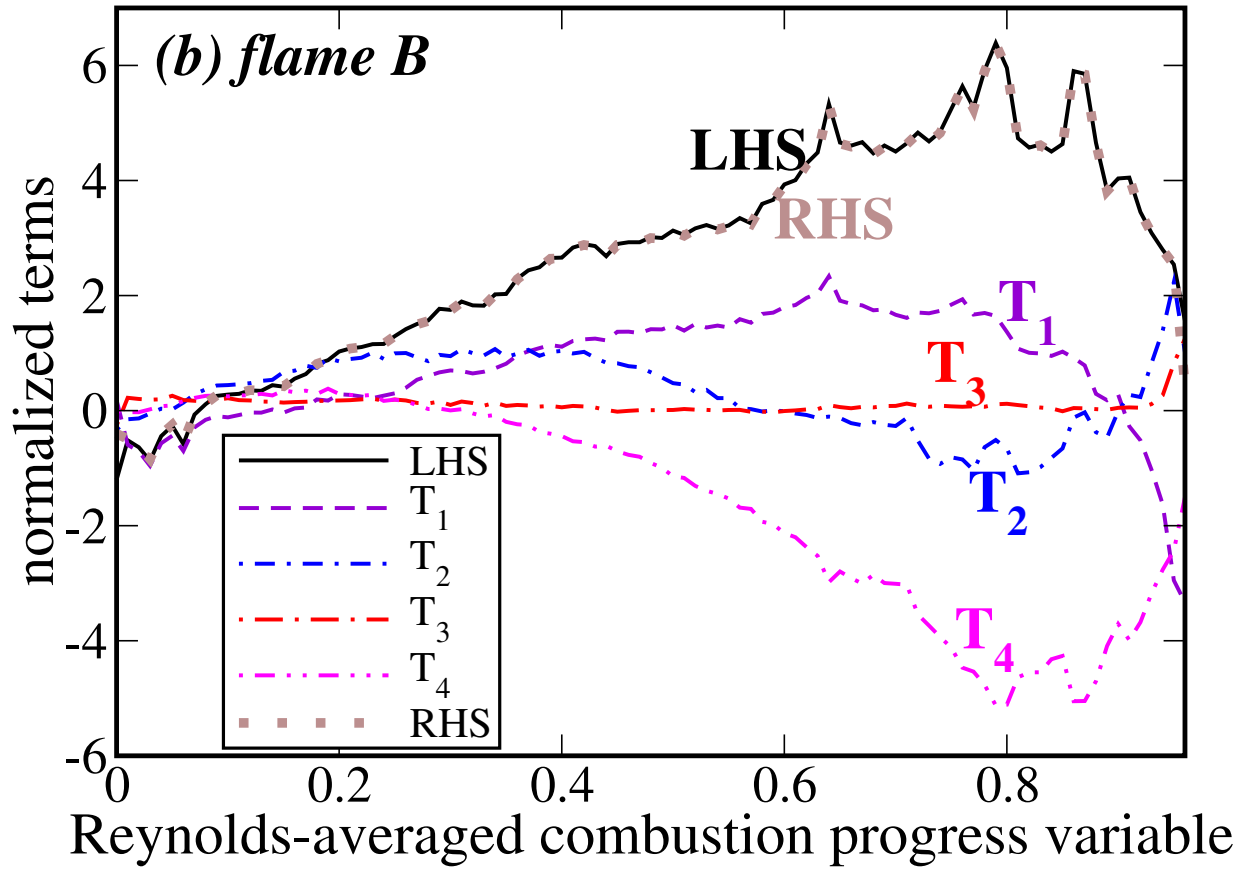
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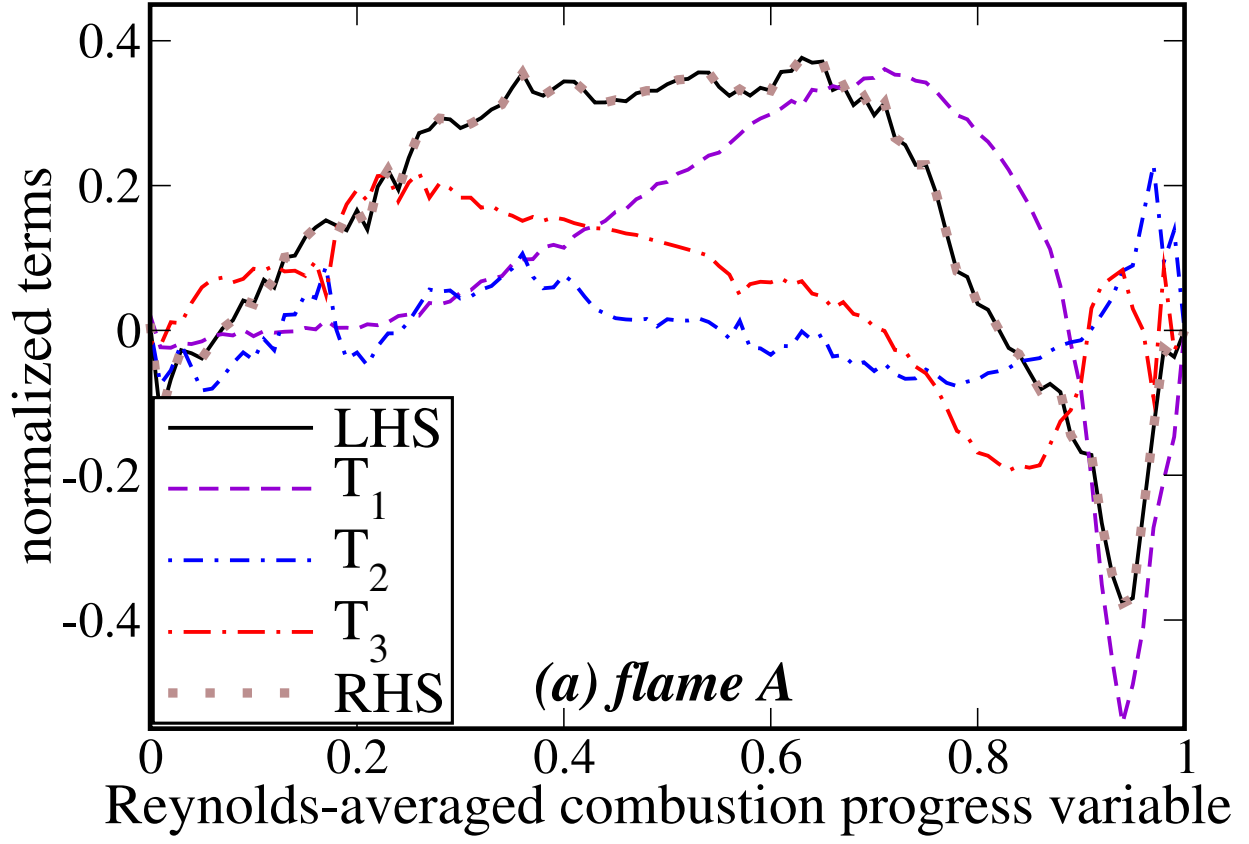
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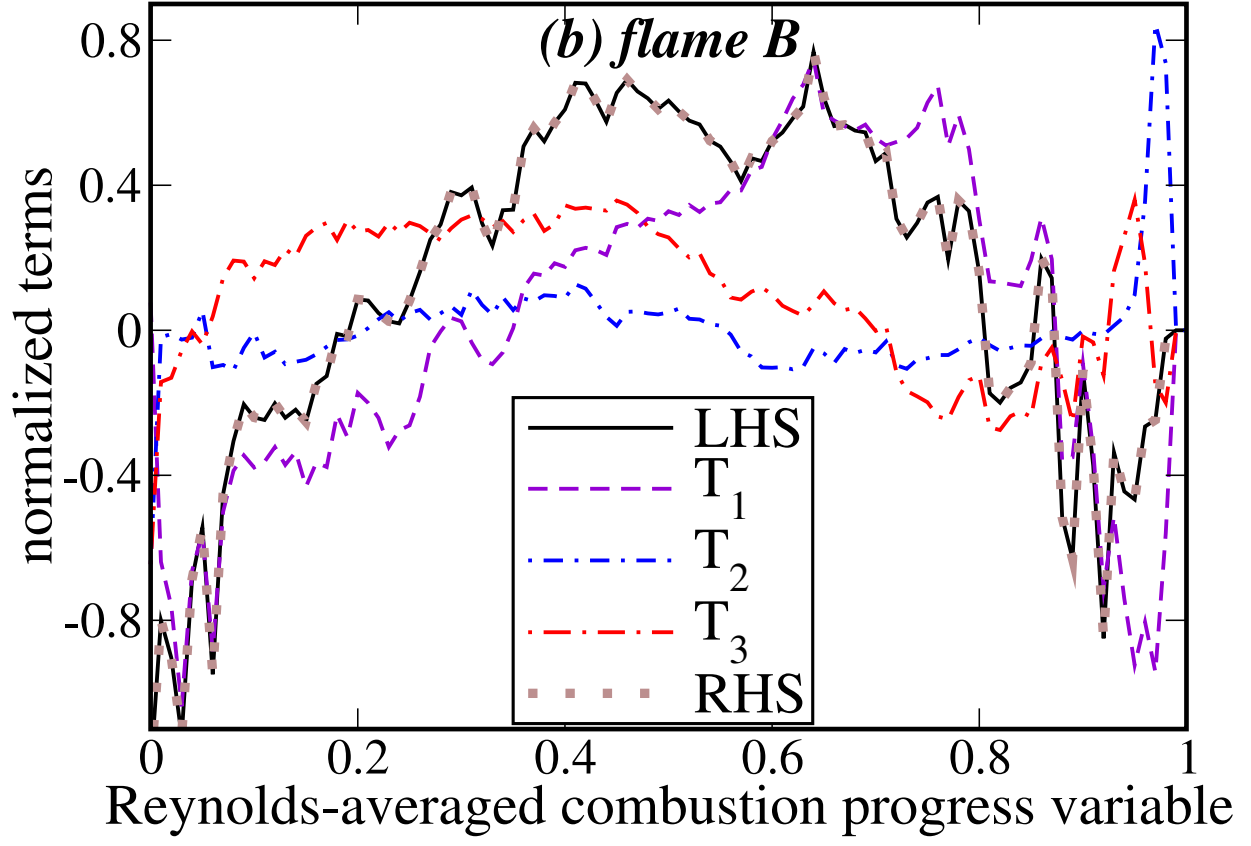
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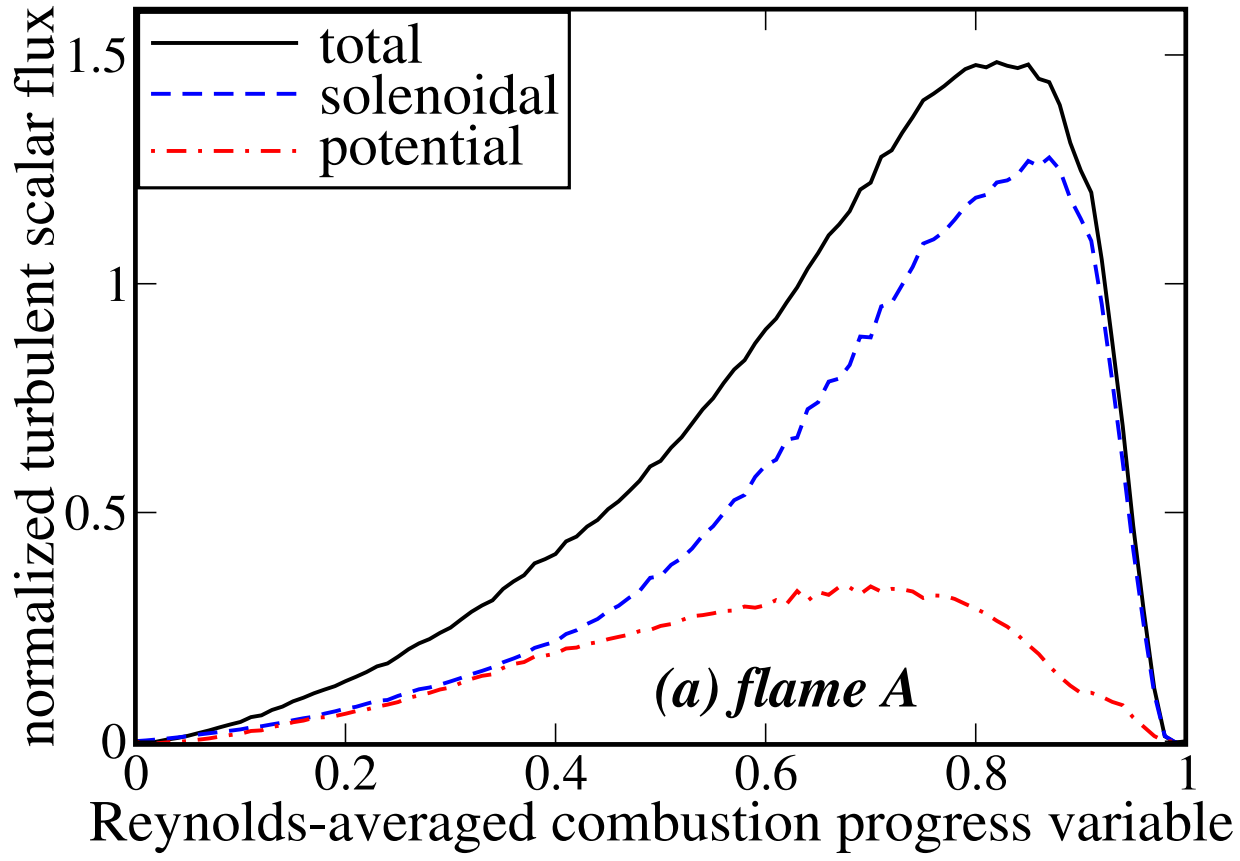
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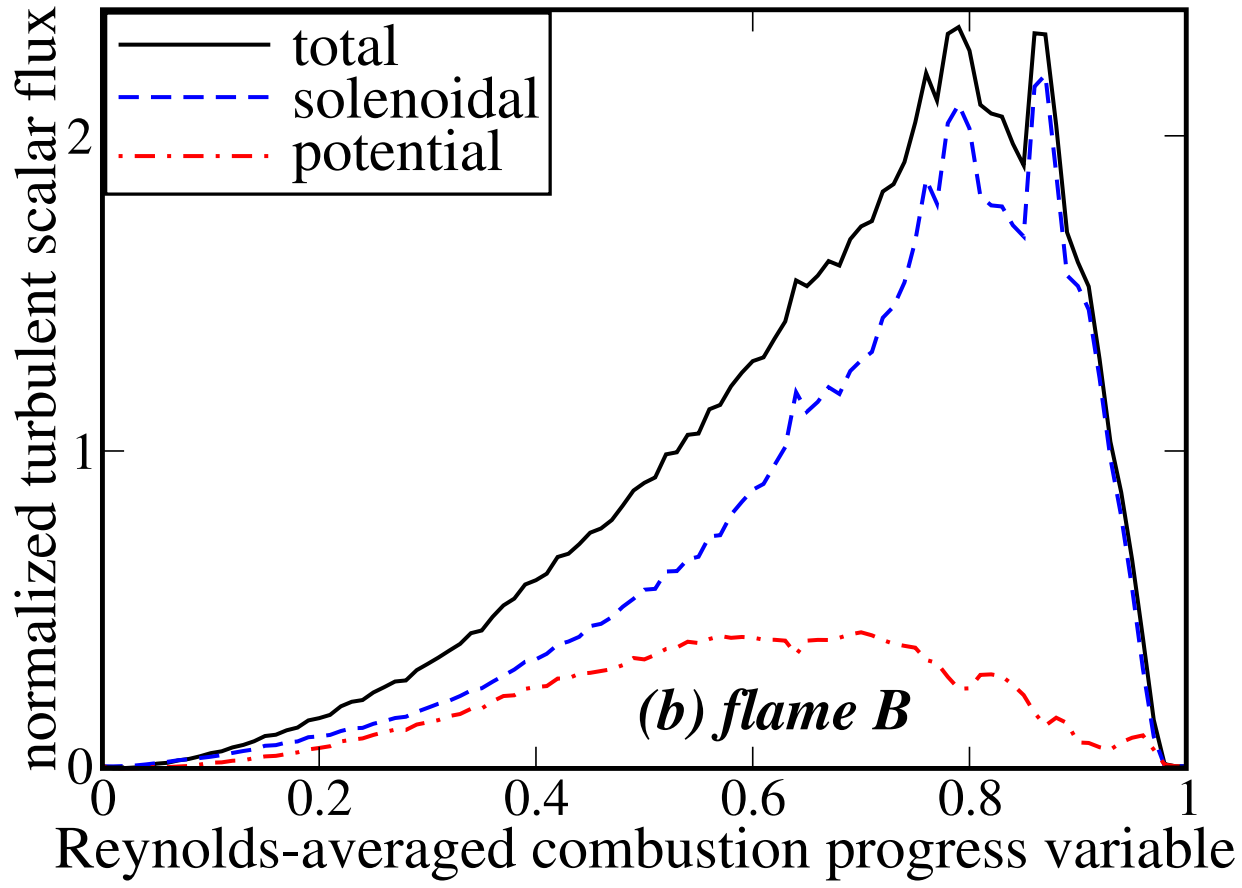
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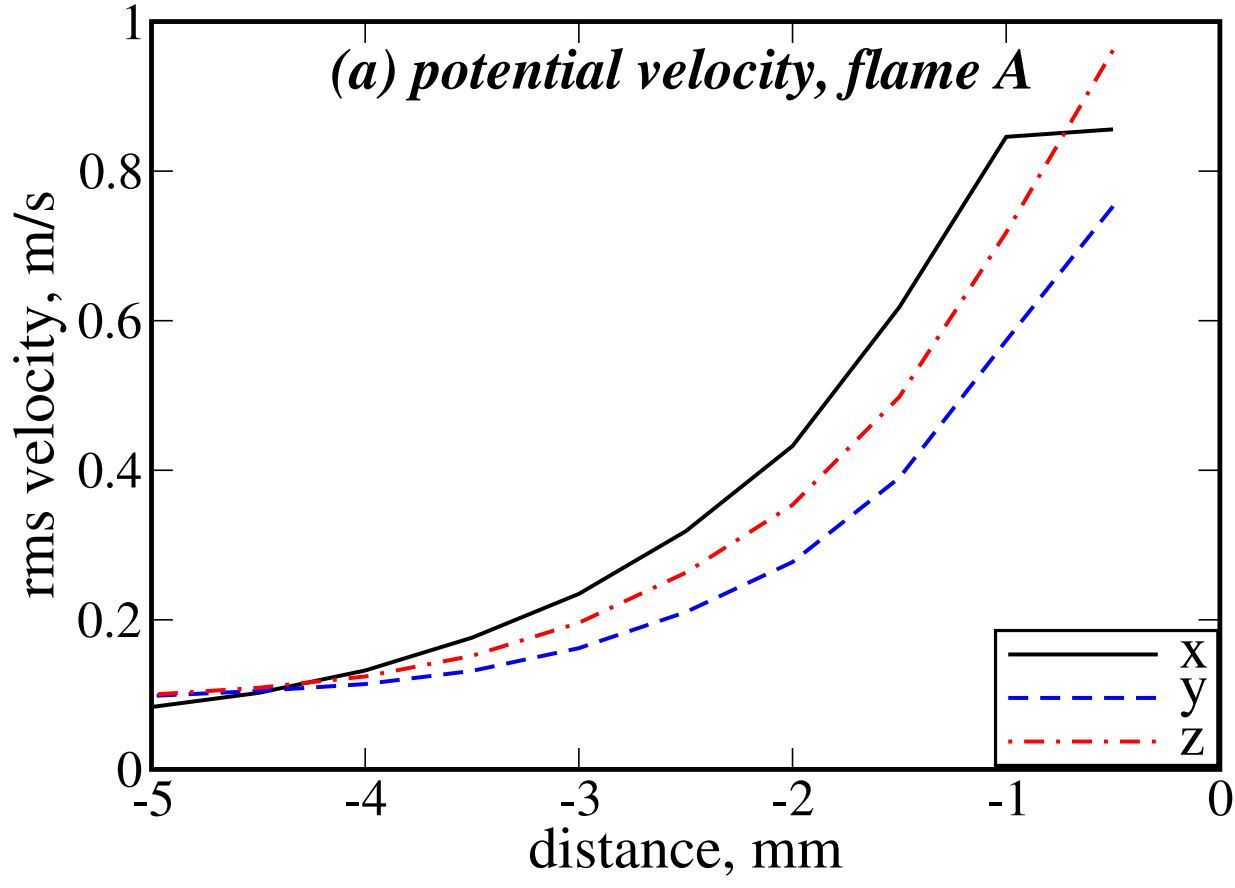
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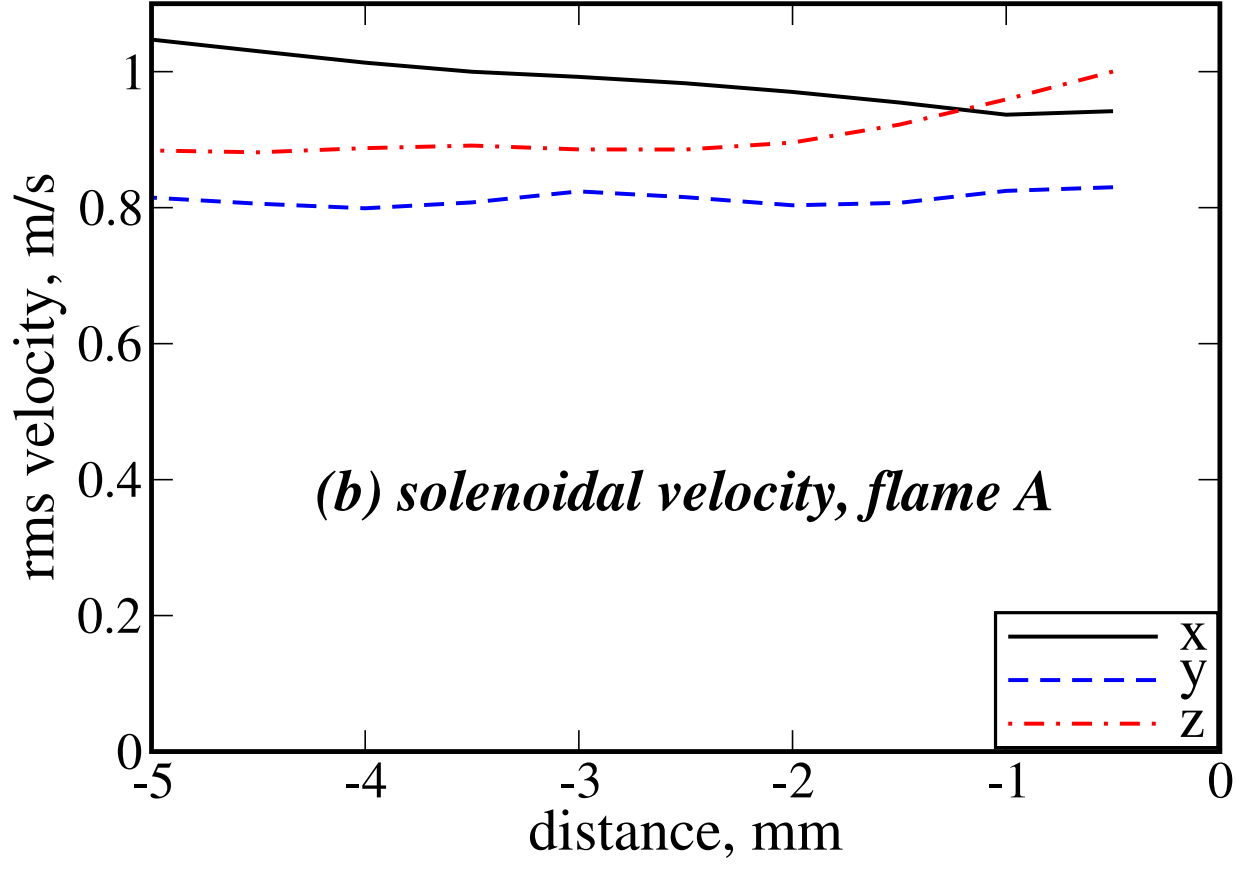
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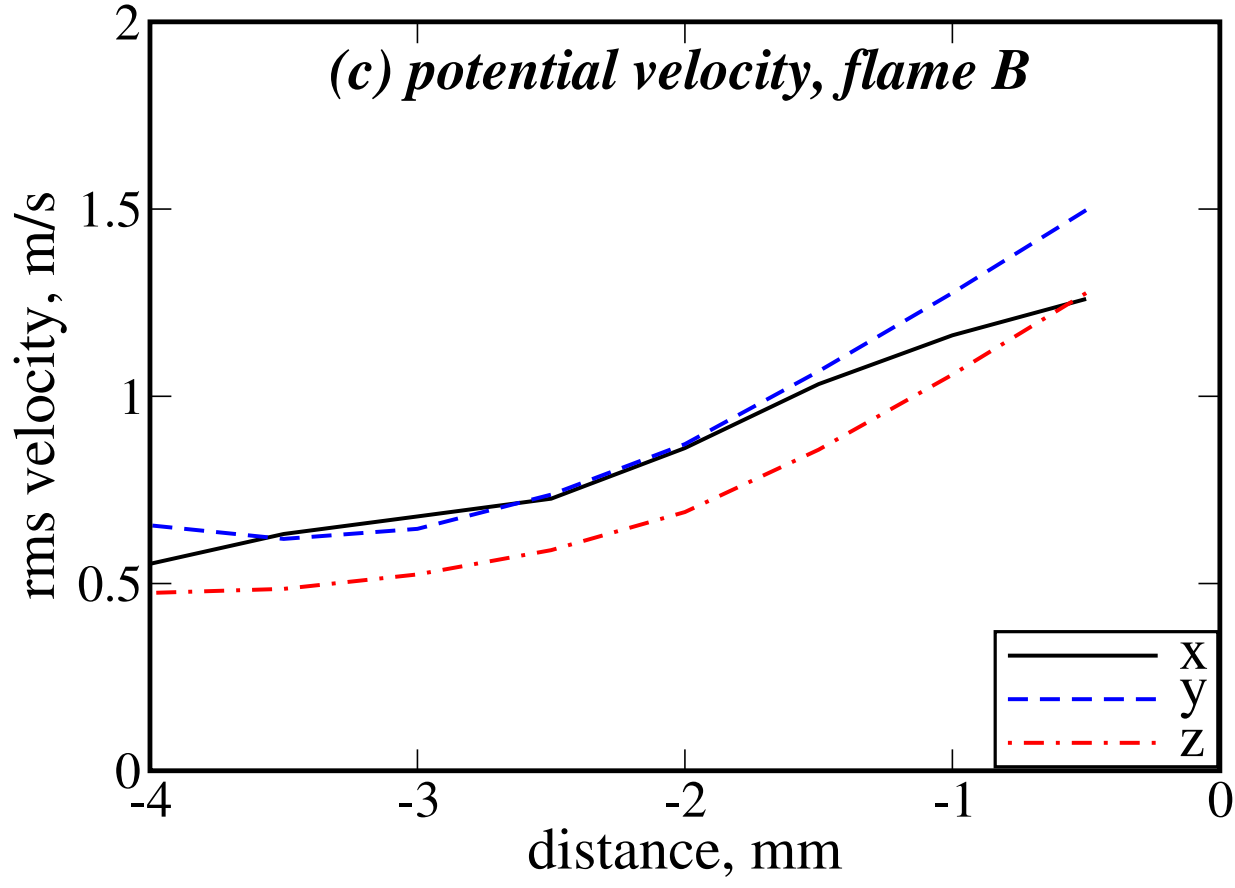
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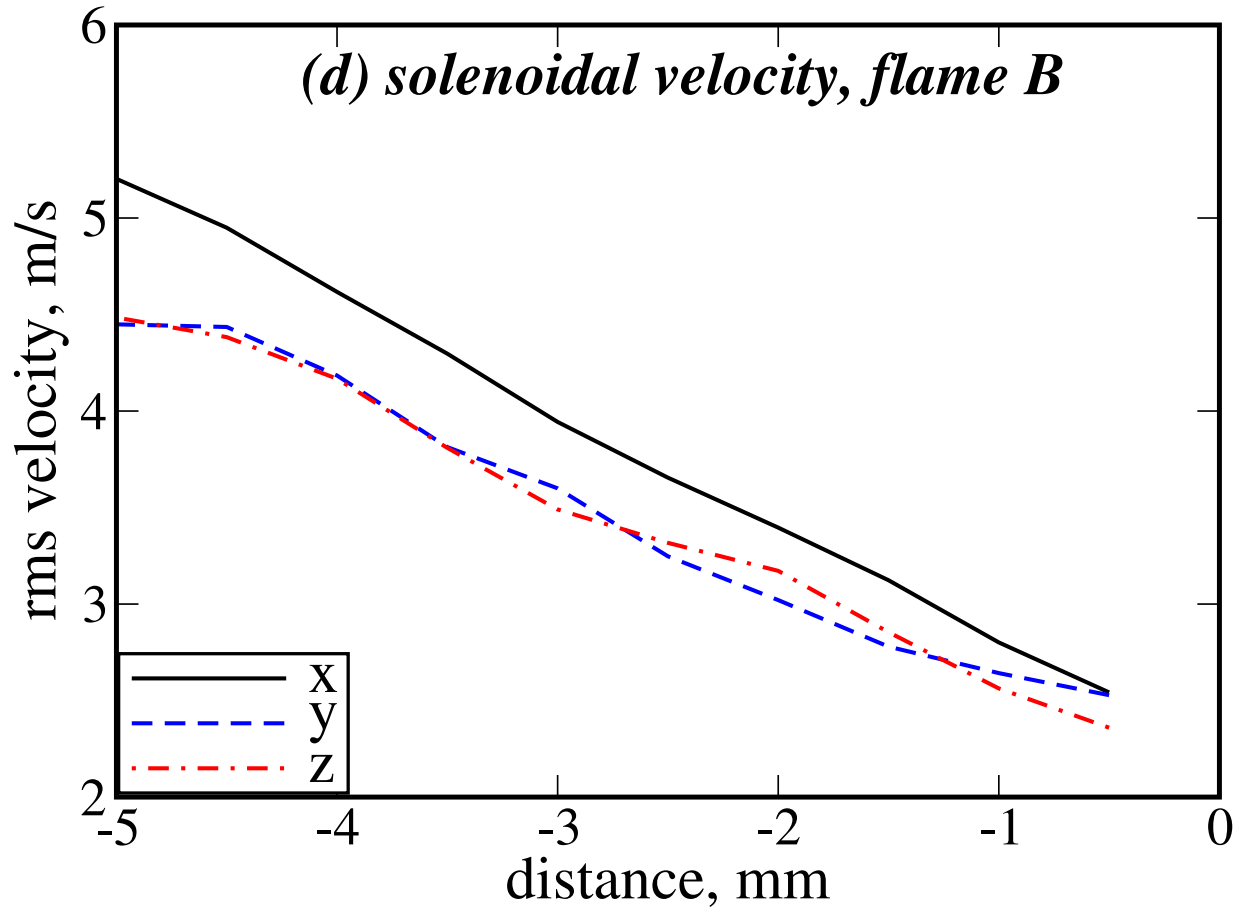
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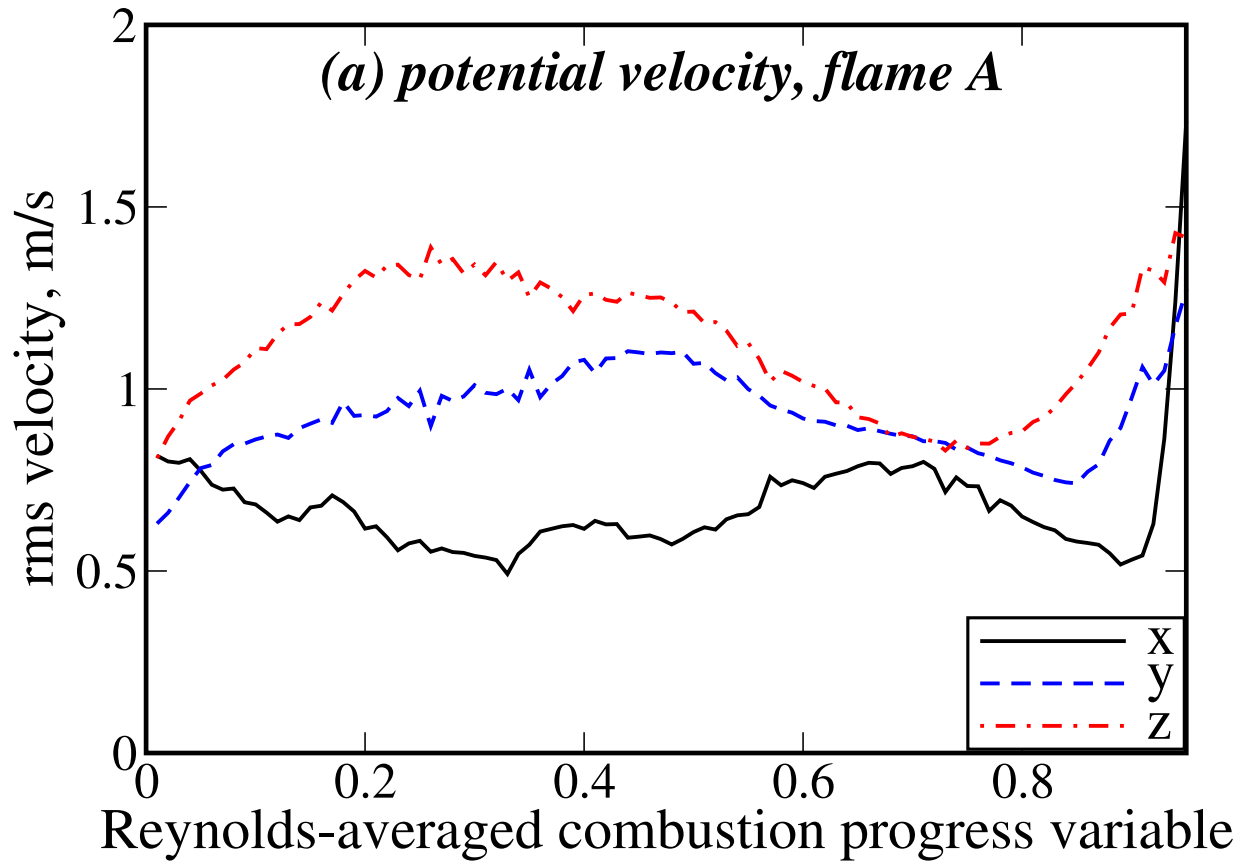
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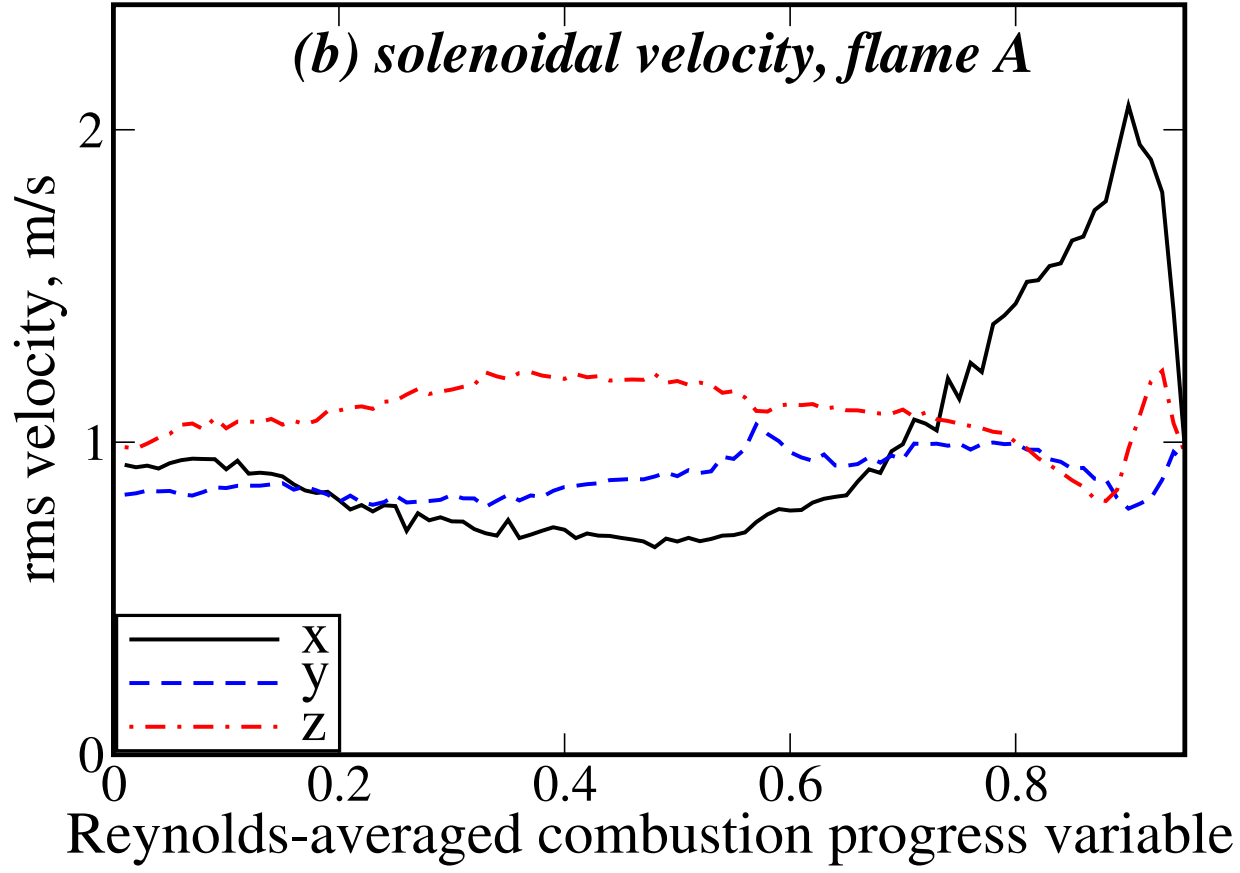
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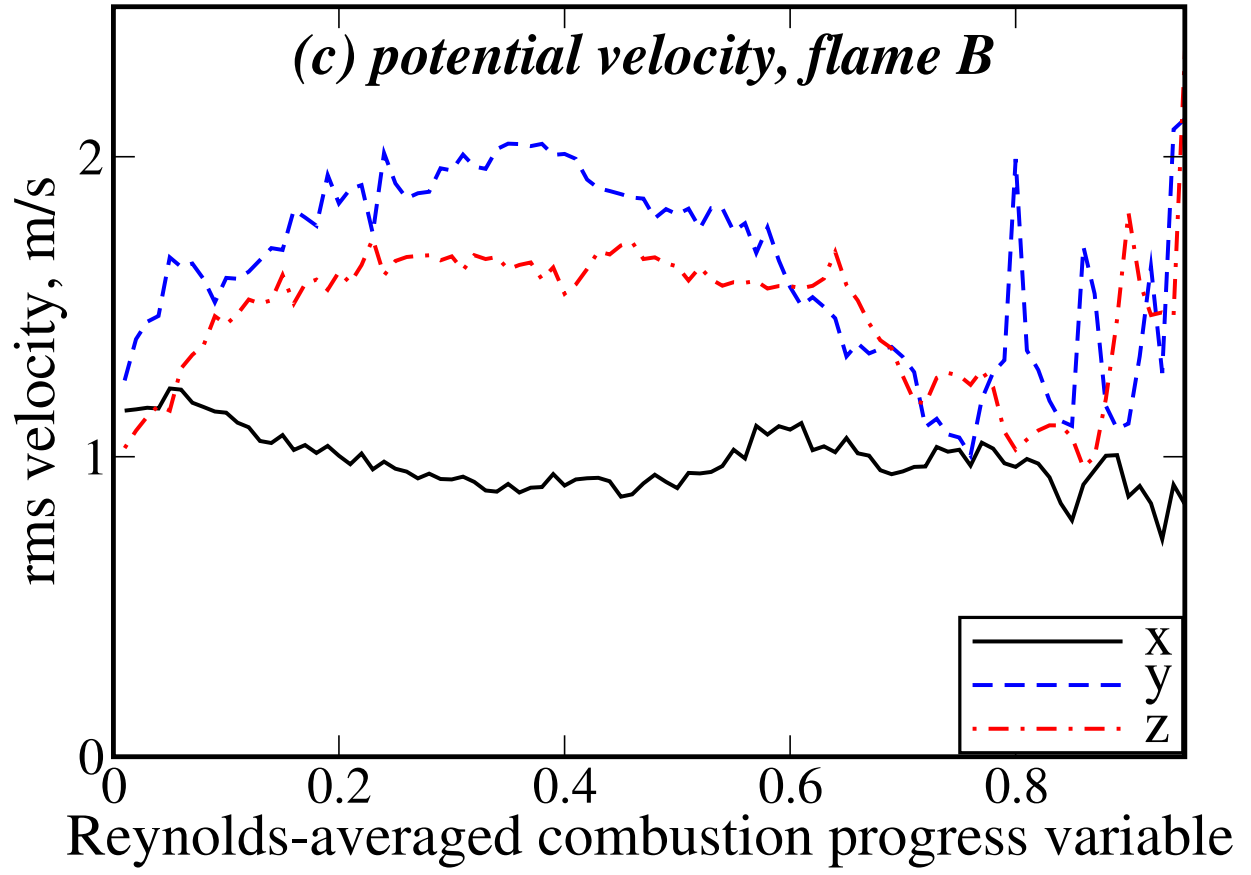
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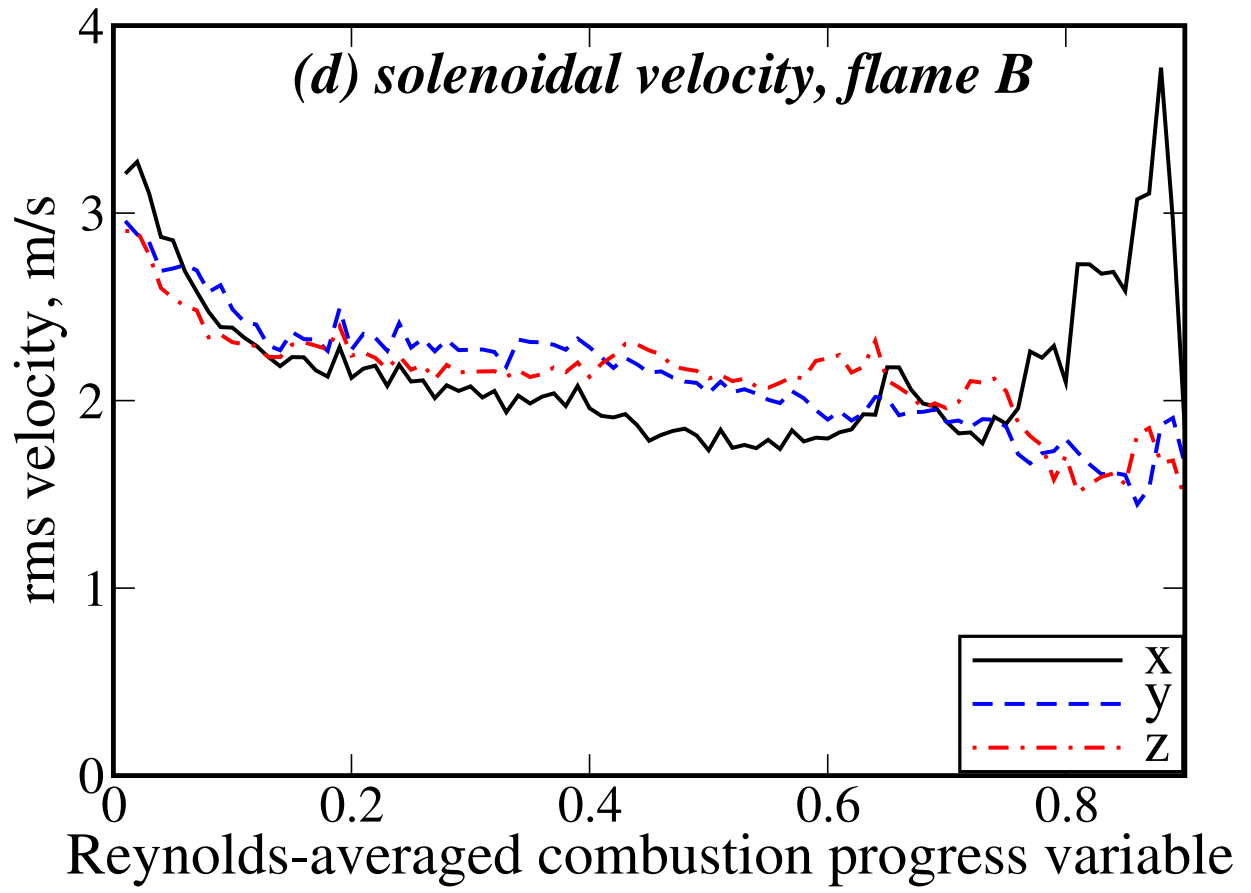
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