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1 **Effects of thermal expansion on moderately intense turbulence in**
 2 **premixed flames**

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13 **Abstract**

14 The study aims at analytically and numerically exploring the influence of combustion-induced thermal
 15 expansion on turbulence in premixed flames. In the theoretical part, contributions of solenoidal and
 16 potential velocity fluctuations to the unclosed component of the advection term in the Reynolds-
 17 averaged Navier-Stokes equations are compared and a new criterion for assessing the importance of
 18 the thermal expansion effects is introduced. The criterion highlights a ratio of the dilatation in the
 19 laminar flame to the large-scale gradient of root-mean-square (rms) velocity in the turbulent flame
 20 brush. To support the theoretical study, direct numerical simulation (DNS) data obtained earlier from
 21 two complex-chemistry, lean H₂-air flames are analyzed. In line with the new criterion, even at
 22 sufficiently high Karlovitz numbers, results show significant influence of combustion-induced potential
 23 velocity fluctuations on the second moments of the turbulent velocity upstream of and within the flame
 24 brush. In particular, the DNS data demonstrate that (i) potential and solenoidal rms velocities are
 25 comparable in the unburnt gas close to the leading edge of the flame brush and (ii) potential and
 26 solenoidal rms velocities conditioned to unburnt gas are comparable within the entire flame brush.
 27 Moreover, combustion-induced thermal expansion affects not only the potential velocity, but even the
 28 solenoidal one. The latter effects manifest themselves in a negative correlation between solenoidal
 29 velocity fluctuations and dilatation or in the counter-gradient behavior of the solenoidal scalar flux.
 30 Finally, a turbulence-in-premixed-flame diagram is sketched to discuss the influence of combustion-
 31 induced thermal expansion on various ranges of turbulence spectrum.

32 **I. INTRODUCTION**

33 Since the pioneering work by Karlovitz et al.¹ and Libby and Bray,² effects of thermal
 34 expansion on turbulence (e.g., so-called flame-generated turbulence¹) and turbulent scalar
 35 transport (e.g., so-called counter-gradient diffusion²) in premixed flames have long been a
 36 challenging research subject.³⁻¹⁵ Numerical studies reviewed elsewhere¹⁶⁻¹⁹ 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^{11,20-23} (DNS) and experimental^{24,25} 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 Bray²⁶ 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 α 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 δ_L .²⁷ Since a widely accepted model of α 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, Bilger²⁸ has hypothesized that such an influence is significant if the
 55 magnitude τ_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 scales²⁵,
 62 respectively; ν 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^{30,31}
 70 of two stoichiometric H₂-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,²⁸ larger eddies from the inertial range of Kolmogorov
 74 turbulence²⁹ may also be affected by the thermal expansion in flames.^{10,32} In particular,
 75 O'Brien et al.³² have theorized that thermal energy released by combustion and transformed

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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 τ_f . MacArt and Mueller¹⁰ 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:

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

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; τ_{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 hold³³

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

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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

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

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

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

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/δ_ℓ or less. Here,
 131 δ_ℓ is the mean flame brush thickness.

132 To estimate the order of magnitude of the last term, let us, first, similarly to Bilger,²⁸ 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.^{34,35} DNS data reported
 136 in Sect. IV support this assumption. It is also worth remembering that eventual decrease in

137 dilatation due to local flame broadening by small-scale turbulent eddies may be
 138 counterbalanced by (i) an increase in the dilatation magnitude due to straining of the local
 139 flame by larger turbulent eddies³⁶ and (ii) differential diffusion effects,³⁷ which are discussed
 140 in detail elsewhere.³⁸

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

145 Thus, the fourth term on the RHS of Eq. (6) is expected to be on the order of $u'\theta =$
 146 $u'(\sigma - 1)\tau_f^{-1}$ bearing in mind that \mathbf{u}'_s and \mathbf{u}' are of the same order when the thermal expansion
 147 effects become relatively weak (close to the boundary we seek for). Therefore, the considered
 148 term, which involves potential velocity fluctuations, should play an important role unless the
 149 dilatation θ is much smaller than u'/δ_t . Contrary to Eq. (2), this newly introduced criterion
 150 compares θ with the large-scale gradient of the rms turbulent velocity in the mean flame
 151 brush, rather than with the small-scale velocity gradient in Kolmogorov eddies. As the former
 152 gradient is significantly smaller, the newly introduced criterion implies importance of thermal
 153 expansion effects in a wider domain of flame characteristics.

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

$$156 \quad Da_{cr}^{-1} = (\sigma - 1) \frac{\delta_t}{L}, \quad (7)$$

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

158 The same criterion can be obtained in a different way. Let us consider the following well-
 159 known Reynolds-averaged transport equation^{16-19,26,35}

$$160 \quad \frac{\partial \bar{c}}{\partial t} + \overline{u_k \frac{\partial c}{\partial x_k}} = \frac{1}{\rho} \overline{\frac{\partial q_{c,k}}{\partial x_k}} + \frac{1}{\rho} \overline{\dot{\omega}_c} \quad (8)$$

161 for a combustion progress variable c , which characterizes mixture state in a flame and varies
 162 from zero in unburnt reactants to unity in the equilibrium adiabatic combustion products.
 163 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
 164 creation. The convection term, i.e., the second term on the LHS of Eq. (8), reads

$$165 \quad \overline{u_k \frac{\partial c}{\partial x_k}} = \overline{\frac{\partial u_k c}{\partial x_k}} - c \overline{\frac{\partial u_k}{\partial x_k}} = \overline{\frac{\partial u_{s,k} c}{\partial x_k}} + \overline{\frac{\partial u_{p,k} c}{\partial x_k}} - c \overline{\frac{\partial u_{p,k}}{\partial x_k}}. \quad (9)$$

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

169 In Eq. (7), the thickness δ_t is unknown *a priori*. Various experimental³⁹⁻⁴² and DNS^{34,43-45}
 170 data show that $\delta_t/L > 1$. Therefore, Da_{cr} should be less than $(\sigma - 1)^{-1} = O(10^{-1})$.
 171 Moreover, DNS data^{43,44} indicate that mean thickness of a fully-developed turbulent premixed
 172 flame, i.e., a turbulent premixed flame propagating at a constant speed and having a constant
 173 thickness, scales as $\delta_{t,\infty}/L \propto (u'/S_L)^{1/3}$ in moderately intense ($u'/S_L \leq 10$, $Da > 0.2$)
 174 turbulence, whereas a subsequent DNS study³⁴ has yielded $\delta_{t,\infty}/L \propto Da^{-1/2}$ at $Da < 0.1$.
 175 Here, the subscript ∞ refers to the fully-developed flame. Let us invoke the latter scaling for
 176 δ_t/L , because Eq. (7) implies that a small $Da < O(10^{-1})$ is required for the thermal
 177 expansion effects to be of minor importance in turbulent flames. We arrive at

$$178 \quad Da_{cr} = (\sigma - 1)^{-2} \quad (10)$$

179 by disregarding numerical factors of unity order.

180 In the following the thickness $\delta_t = (T_b - T_u)/\max|\nabla \bar{T}|$ will be extracted from the DNS
 181 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

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

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

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

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 $\tilde{u}_i = \overline{u_i + u'_i} = \bar{u}_i + \tilde{u}'_i$ 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

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

208 III. NUMERICAL SIMULATIONS

209 A. DNS conditions

210 As the DNS attributes and data were reported earlier,^{11,15,46-48} 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 $\Phi=0.7$) H_2 -air turbulent flames were investigated by (i)
 213 adopting a detailed (9 species, 23 reversible reactions) chemical mechanism⁴⁹ 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 H_2 -air flames and to significantly
 217 increase turbulent burning velocity, as reviewed elsewhere,³⁸ differential diffusion was
 218 shown^{50,51} 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.

220

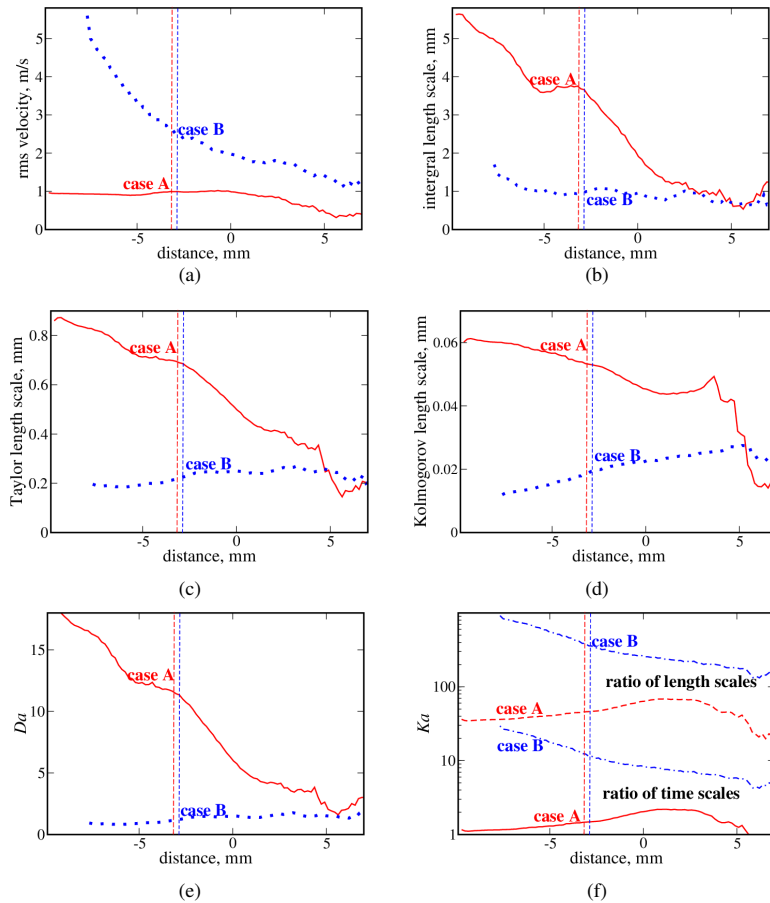


FIG. 1. Axial variations of turbulent flame characteristics conditioned to unburned mixture in flames A (red lines) and B (blue lines). Vertical dotted-dashed lines show the flame-brush leading edge, i.e., planes characterized by $\bar{c}(\xi) = 0.05$. (a) rms turbulent velocity u' , (b) integral length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

221 Two cases A and B, characterized by two different values of the inlet rms velocity, with all
 222 other things being equal, were studied. Variations of the major turbulence characteristics along
 223 the x -axis in these two cases are shown in Fig. 1. Here, the distance ξ is counted from a
 224 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; $\tau_K = (v_u / \langle \varepsilon | c < 0.02 \rangle)^{1/2}$ and $\eta_K =$
 230 $(v_u^3 / \langle \varepsilon | c < 0.02 \rangle)^{1/4}$; $\lambda = 15 v_u u'^2 / \langle \varepsilon | c < 0.02 \rangle$ is Taylor microscale; and the local
 231 dissipation rate $\varepsilon = 2 v_u S_{jk} S_{jk}$. A slow decrease in η_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/δ_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;⁵² $Re_T = u'_0 L_T / v_u$; 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

246 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
 247 complex-chemistry case.

248 The criteria introduced in Sect. II, both Eq. (7) and Eq. (10), imply that combustion-induced
 249 thermal expansion can substantially affect the large-scale turbulence characteristics in both
 250 flames A and B. On the contrary, Eq. (2) suggests that the influence of the thermal expansion
 251 on the small-scale turbulence characteristics can be of importance in flame A only, whereas
 252 $Ka > Ka_{cr}^B$ in case B.

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

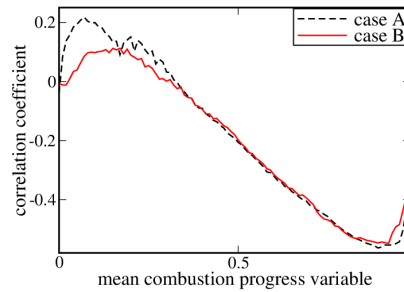
256 **B. Helmholtz-Hodge decomposition**

257 The fluctuating velocity $\mathbf{u}'(\mathbf{x}, t)$ was decomposed into solenoidal and potential components
 258 $\mathbf{u}'_s(\mathbf{x}, t)$ and $\mathbf{u}'_p(\mathbf{x}, t)$ by using two methods: (i) conventional³³ HHD and (ii) natural^{53,54}
 259 decompositions. To do so, algorithms that were applied earlier by the present authors to
 260 velocity fields obtained from weakly turbulent single-step chemistry flames^{55,56} and from
 261 flames¹⁵ A and B were adopted. The reader interested in a detailed discussion of these
 262 algorithms is referred to the latter paper.¹⁵ Since the earlier results yielded by the two
 263 decompositions were hardly distinguishable within flame brushes,⁵⁵ we will report results
 264 obtained using the former method only.

265 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
 266 $\nabla \times \mathbf{u}''_p \neq 0$.

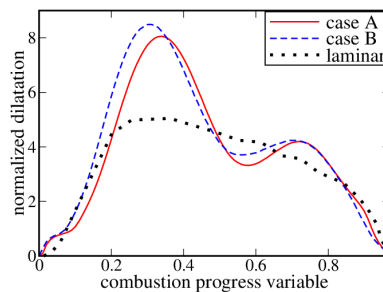
267 **IV. NUMERICAL RESULTS AND DISCUSSION**

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



272

273 **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} .



274

275 **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
 276 dependence of $\nabla \cdot \mathbf{u}$ on c in the counterpart laminar flame.

277 More specifically, Fig. 3 shows that the conditioned dilatation $\langle \nabla \cdot \mathbf{u} | c \rangle$ is indeed on the
 278 order of $\nabla \cdot \mathbf{u}(c)$ in the laminar flame, while the former can be larger than the latter. A similar
 279 quantitative difference was reported in earlier DNS studies.^{36,37} 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.⁵⁷ 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.^{50,51} 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.

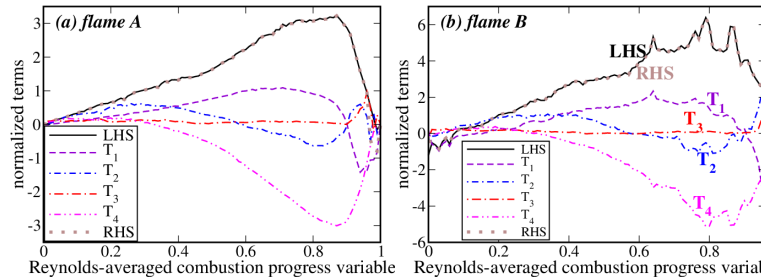
292 Figure 4 shows variations of all terms in Eq. (6) within mean flame brushes. Note that the
 293 almost perfect agreement between the LHS and RHS of this equation in both cases, cf. black
 294 solid and brown dotted lines, verifies conservation in the simulations. Contrary to the criterion
 295 given 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,¹⁶⁻¹⁹
 303 i.e., correlation between solenoidal velocity fluctuations and dilatation is predominantly

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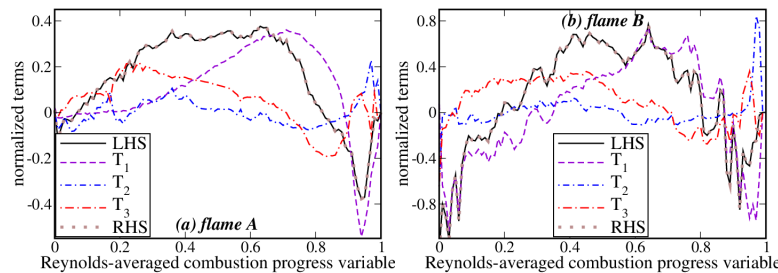
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304 negative (see Fig. 2); but (ii) the RHS of Eq. (6) is positive because it includes T_4 with a minus
 305 sign.



306
 307 **FIG. 4.** Various terms in Eq. (6), normalized using S_L and δ_L , in flames (a) A and (b) B.

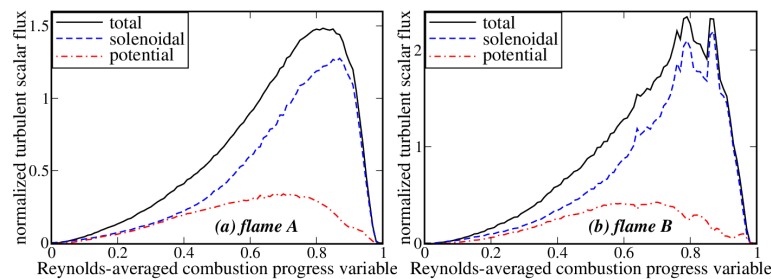
308 Importance of thermal expansion effects is also shown in Fig. 5, which reports various terms
 309 in Eq. (13) for the two statistically one-dimensional planar flames (note almost perfect
 310 matching between the LHS and RHS again). Although the magnitude of the solenoidal term
 311 T_1 is larger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



314
 315 **FIG. 5.** Various terms in Eq. (13), normalized using ρ_u , S_L , and δ_L , in flames (a) A and (b) B.

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

318 dominates at $\bar{c} > 0.5$ on the RHS of Eq. (6), whereas the solenoidal term (T_1) is the most
 319 important term on the RHS of Eq. (13) in the largest parts of the two flame brushes. However,
 320 this result does not mean that the use of Favre-averaged velocities is favorable in solving the
 321 problem of modeling turbulence in flames. The fact that the solenoidal term is the largest term
 322 on the RHS of Eq. (13) at $\bar{c} > 0.5$ does not prove that models developed for solenoidal
 323 incompressible turbulent flows hold for the solenoidal term on the RHS of Eq. (13) in flames.
 324 Rather, combustion-induced thermal expansion can substantially affect not only potential
 325 velocity fluctuations, but also solenoidal turbulence even at high Ka . Two examples follow.
 326 First, Fig. 3 and a large magnitude of term T_4 on the RHS of Eq. (6) (see Fig. 4) show a
 327 well-pronounced negative (at $\bar{c} > 0.4$) correlation between dilatation and solenoidal velocity
 328 fluctuations, thus implying a substantial influence of thermal expansion on the solenoidal
 329 velocity field in the studied flames.



330
 331 **FIG. 6.** Axial turbulent scalar flux normalized using ρ_u and S_L in flames (a) A and (b) B.

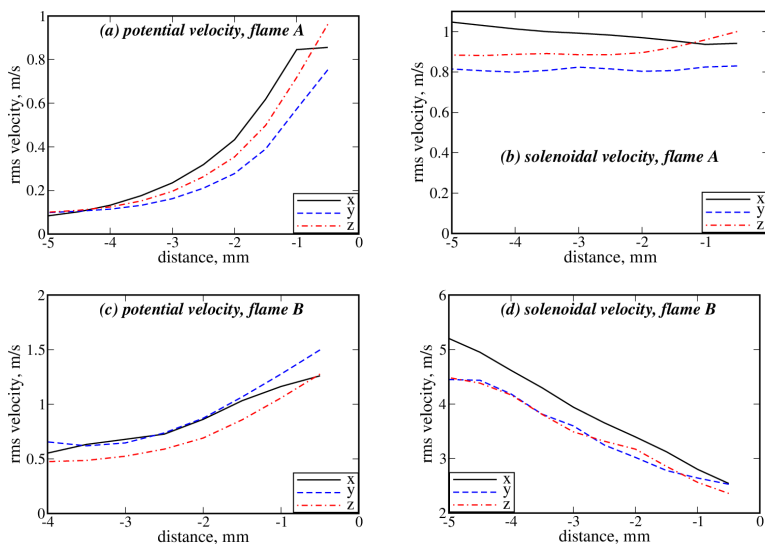
332 Second, Fig. 6 shows that not only the total turbulent scalar flux $\overline{\rho u'' c''}$, but also its
 333 solenoidal and potential components are counter-gradient ($d\bar{c}/dx > 0$ in the studied flames).
 334 The counter-gradient behavior of $\overline{\rho u_s'' c''}$ indicates a substantial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

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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,^{26,27} 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.



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

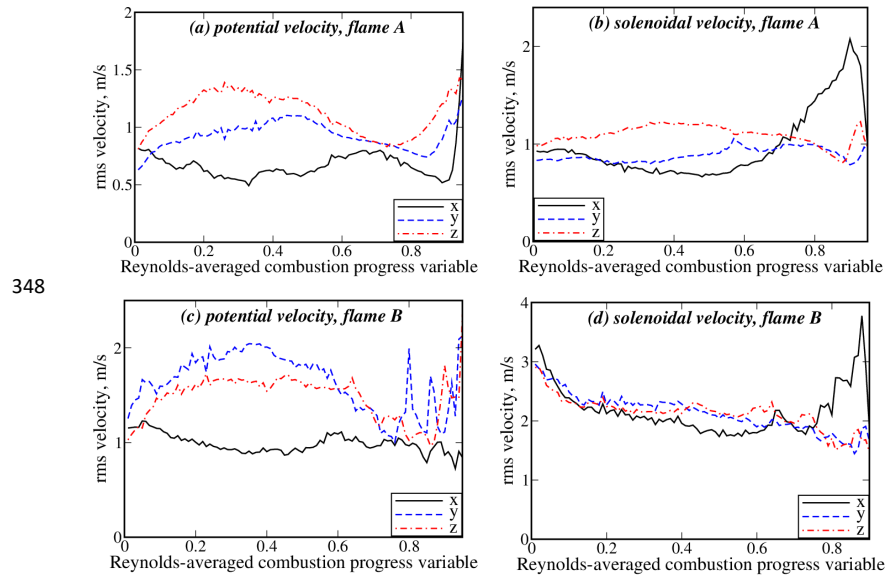


FIG. 8. Variations of (a), (c) potential and (b), (d) solenoidal rms velocities conditioned to unburned mixture, i.e., $\langle u_{i,p}^{\prime 2} | c(\mathbf{x}, t) < 0.01 \rangle^{1/2}$ and $\langle u_{i,s}^{\prime 2} | c(\mathbf{x}, t) < 0.01 \rangle^{1/2}$, respectively, within flames (a)-(b) A and (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 $\langle u_{i,p}^{\prime 2} \rangle^{1/2}$ 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.^{58,59} On the contrary, the solenoidal $\langle u_{i,s}^{\prime 2} \rangle^{1/2}$ 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,⁶⁰⁻⁶² 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 $Da^2Ka^2 \propto Re_t = u'L/\nu$, 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.²⁸ 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 τ_m is shorter than or equal to the laminar flame time scale τ_f . In the inertial
 382 range²⁹ 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.⁶³ 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.⁶⁴ If the energy flux due to combustion
 387 is localized to scales on the order of δ_L ,⁶⁵⁻⁶⁷ the scale l_m should be larger than δ_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.”³²

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,²⁸ let us hypothesize that backscatter may
 397 arise if the dilatation θ 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,¹⁵ 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

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

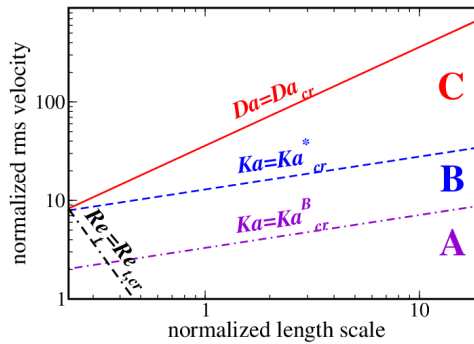
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422 Therefore, $Da_{cr}^* > Da_{cr}$ if $Re_t > (\sigma - 1)^{-5/2} \Gamma^{1/2}$, which holds in a turbulent flow, where
 423 $Re_t \gg 1$. Thus, when compared to Eq. (20), which allows for backscatter in the inertial range,
 424 the newly introduced criterion given by Eq. (10) substantially extends the domain of the
 425 influence of combustion-induced thermal expansion on turbulence in premixed flames to a
 426 lower Damköhler number.

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



434

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.

435 The three criteria given by Eqs. (2), (10), and (20) are plotted in violet dotted-dashed, red
 436 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/δ_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.,³² 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,²⁸ 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,²⁸
 457 rather than contradicting it. The point is that Bilger²⁸ 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 H₂-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^{10,28,32} 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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 489 Supercomputing Laboratory.

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 $20 \times 10 \times 10$ mm³ using a
 495 uniform Cartesian mesh of $512 \times 256 \times 256$ cells. The mesh ensured about ten grid points per
 496 δ_L , with Kolmogorov length scale being larger than cell size Δx . 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.⁷¹ Time
 500 integration was performed adopting an explicit fourth-order Runge-Kutta scheme.⁷¹

501 Along the flame propagation direction, inflow and outflow characteristic boundary
 502 conditions were set using an improved Navier-Stokes characteristic boundary condition
 503 technique.⁷² Other boundary conditions were periodic.

504 A divergence-free, isotropic, homogeneous turbulent velocity field was generated using a
 505 pseudo spectral method⁷³ and adopting the Passot-Pouquet spectrum.⁵² The field was injected
 506 through the inlet (left) boundary and decayed along the mean flow direction (x -axis). At $t =$
 507 0, a pre-computed planar laminar flame structure was embedded into the computational
 508 domain to initialize turbulent flame propagation from right to left along x -axis. Subsequently,
 509 the mean inlet flow velocity was gradually changed to match turbulent flame speed. Results
 510 reported in the present paper were sampled at six different instants in each case, i.e., at $t/t_e =$
 511 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
 512 in case B, where, t_e is the eddy turnover time.

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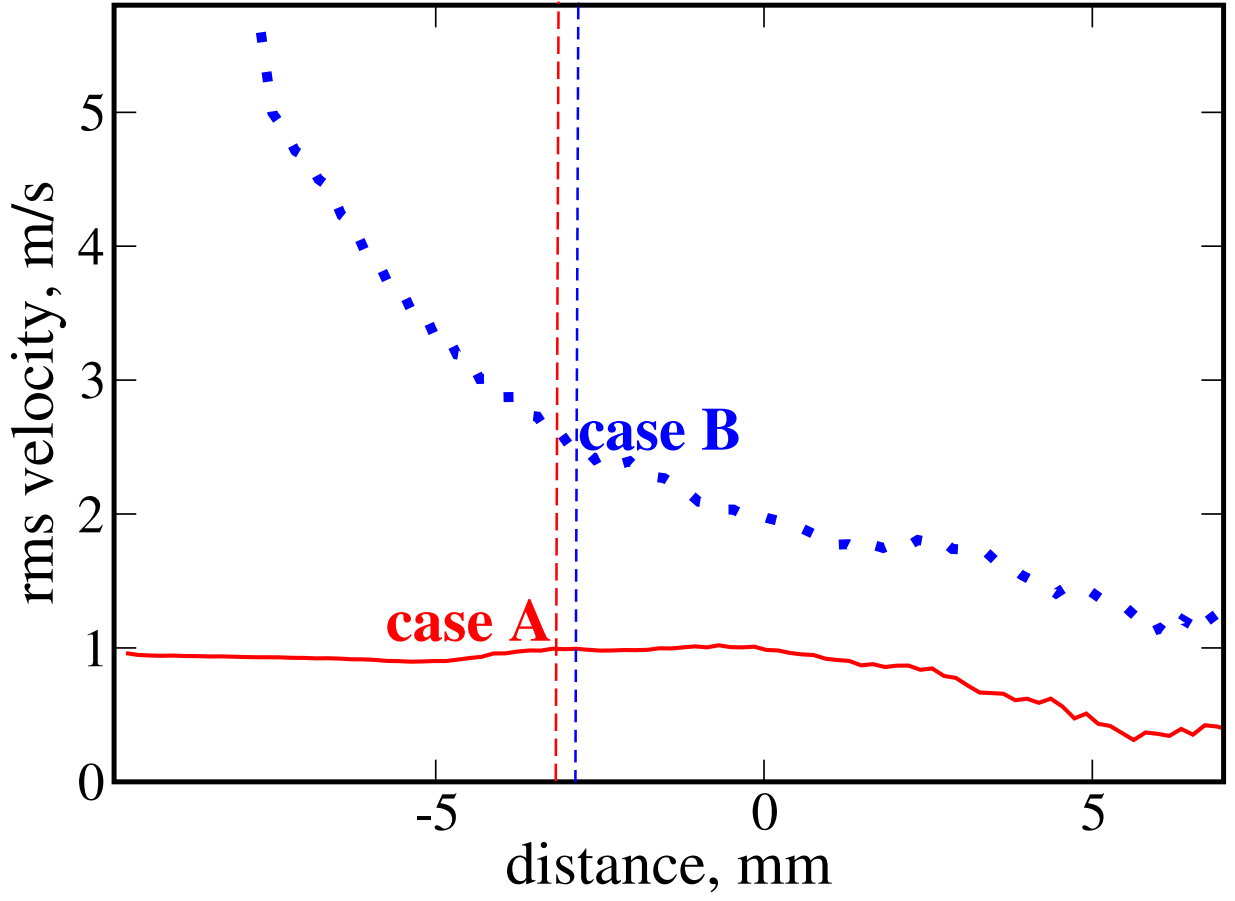
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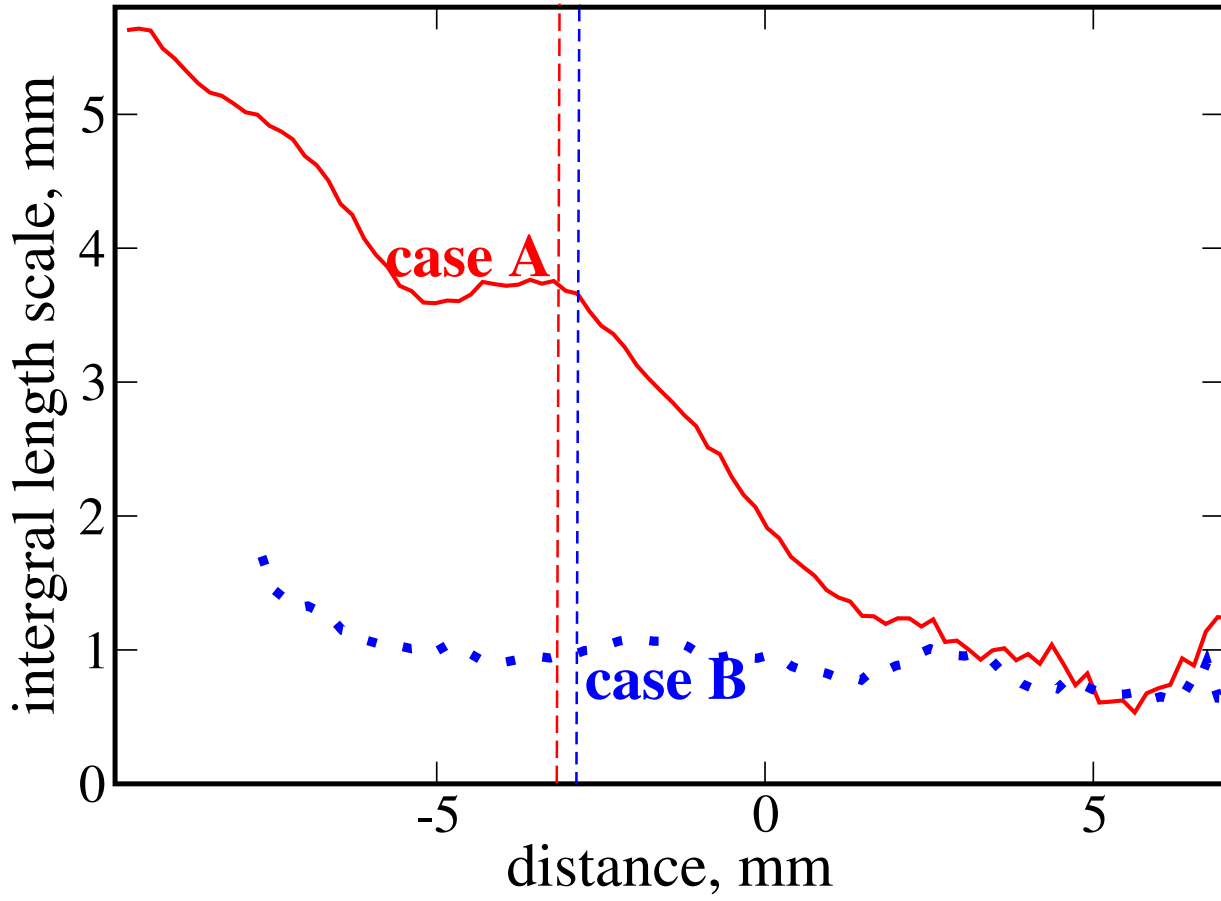
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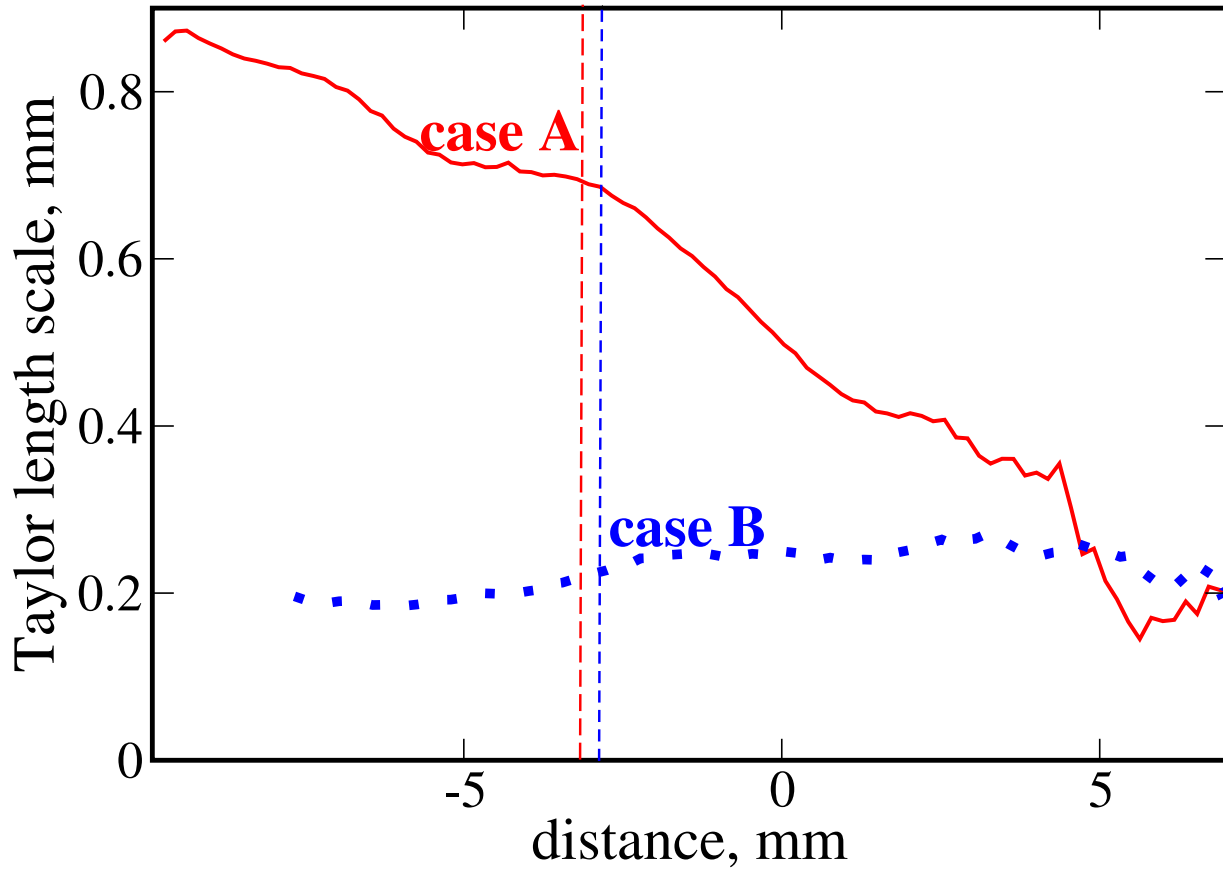
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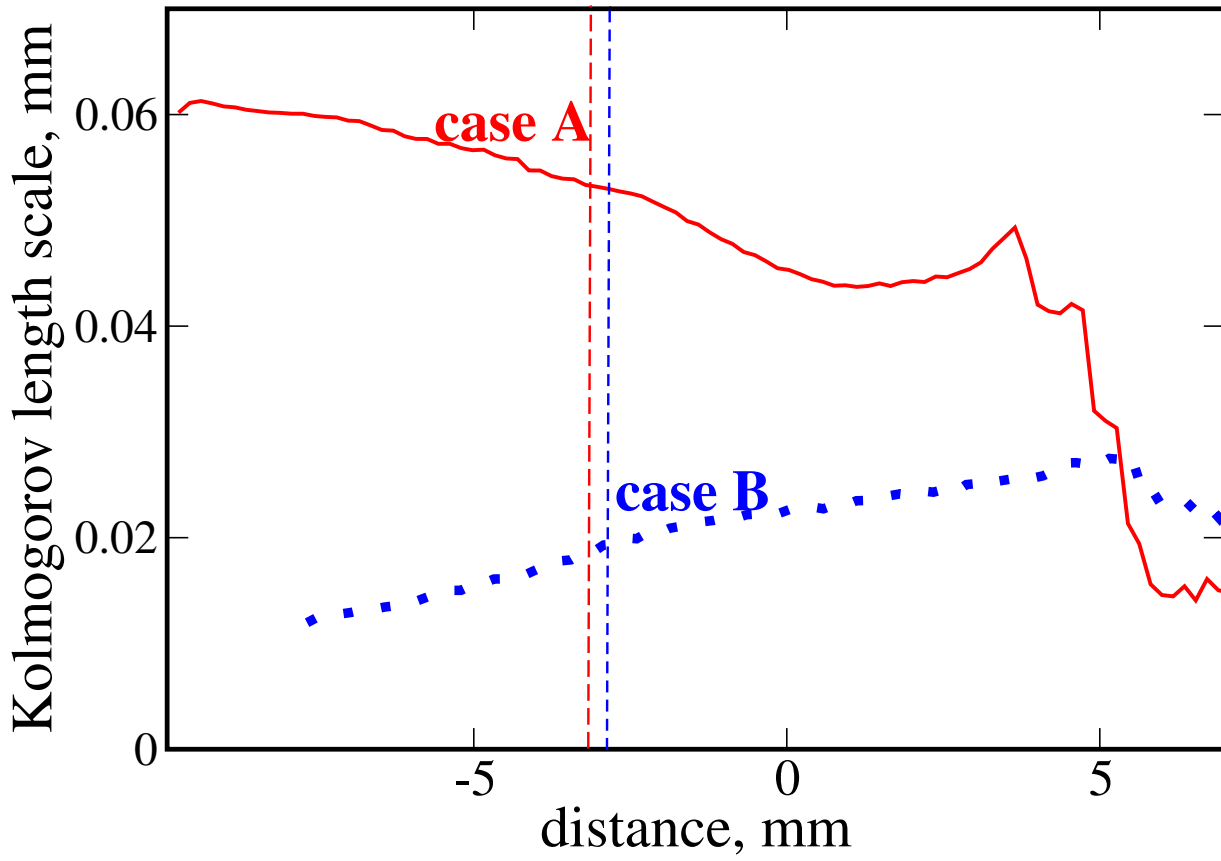
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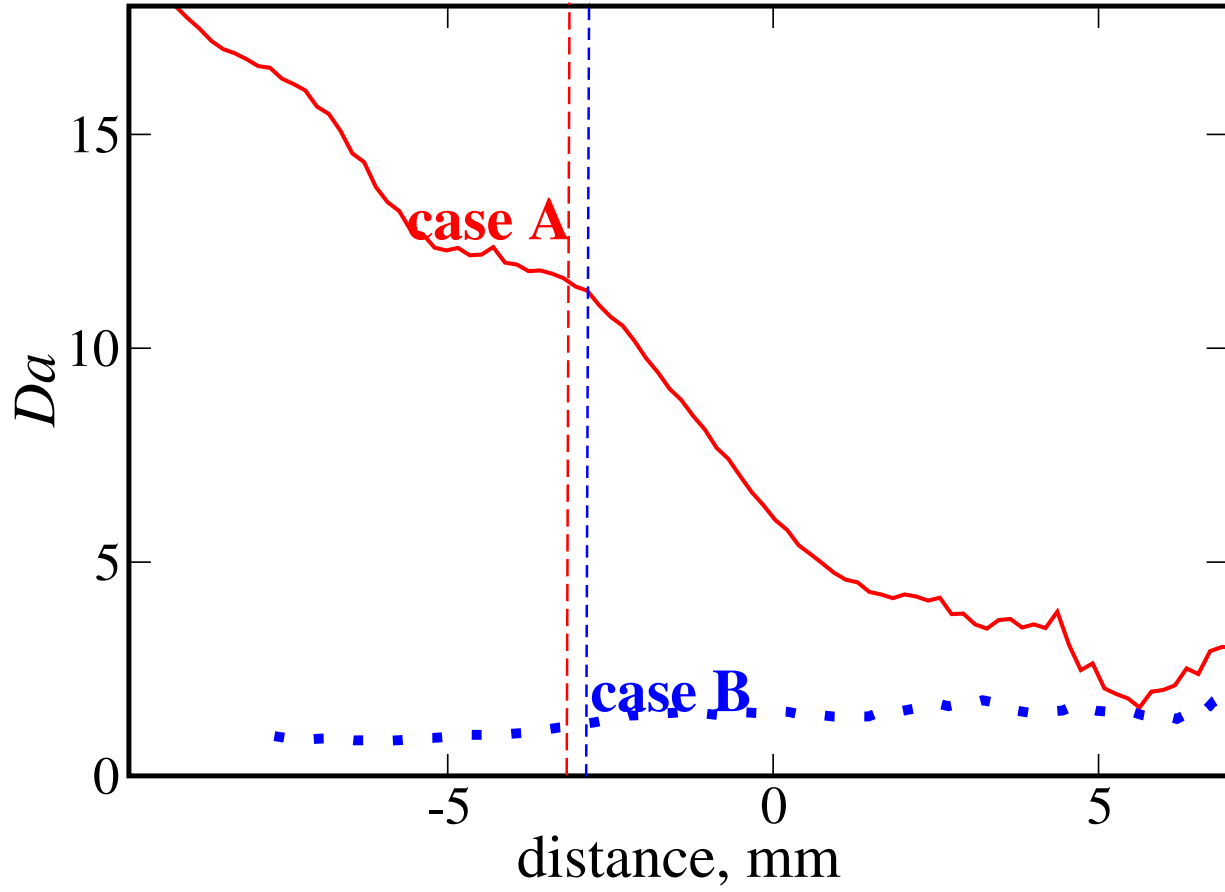
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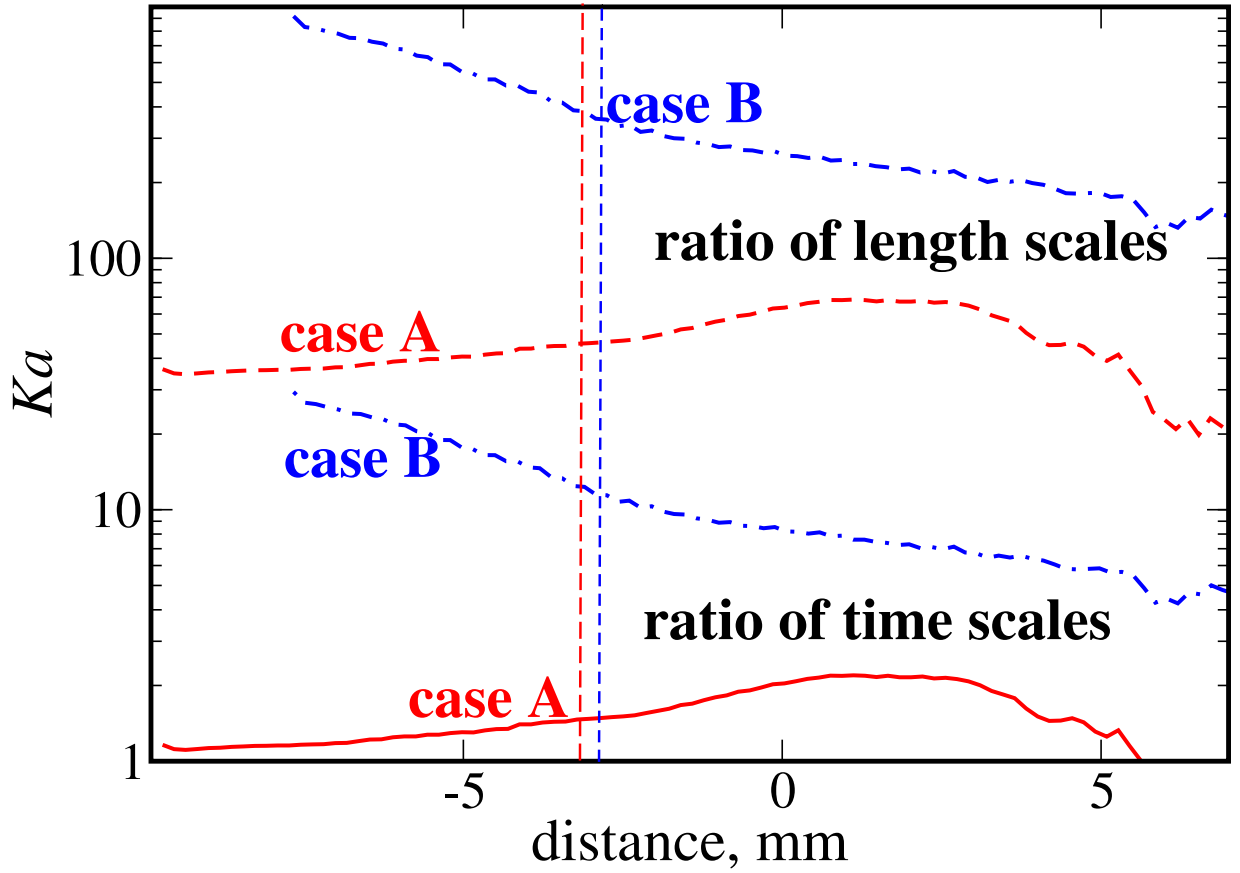


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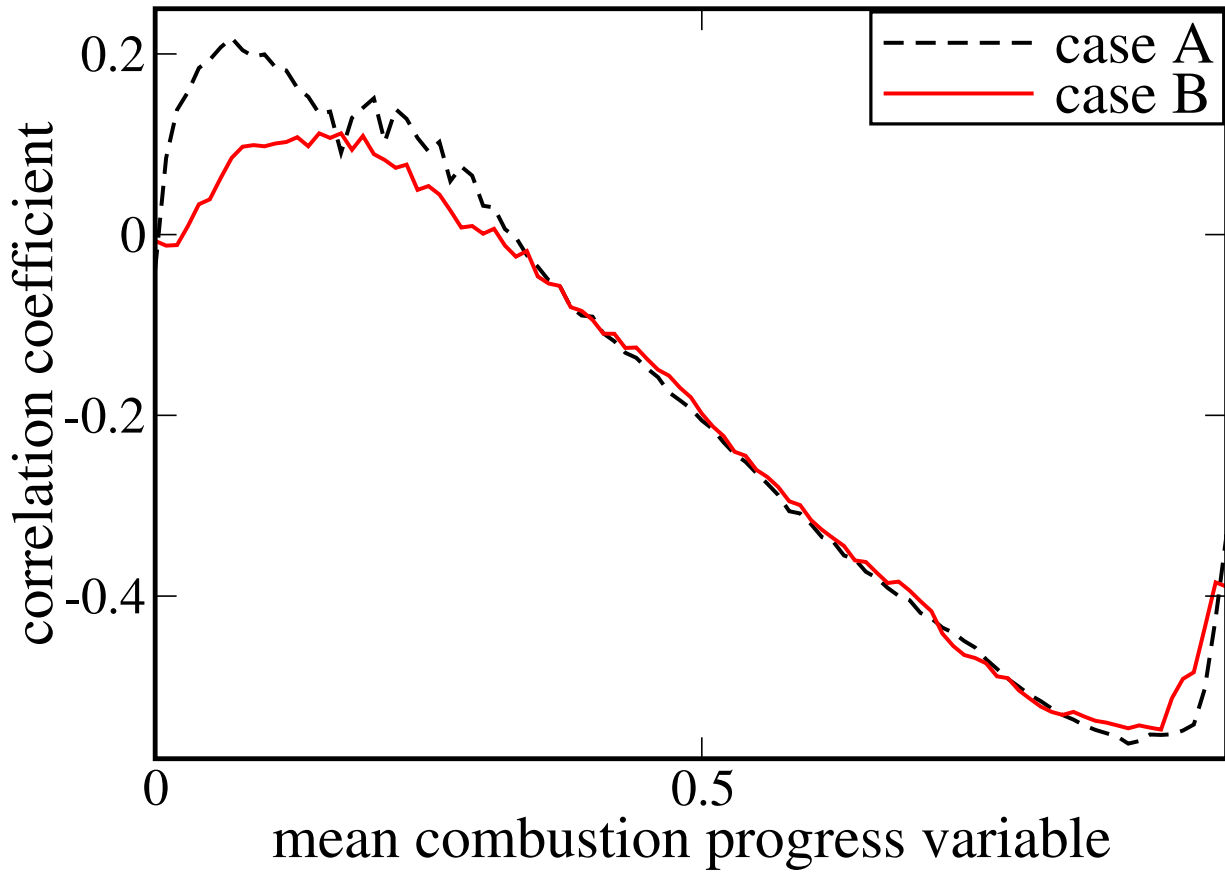


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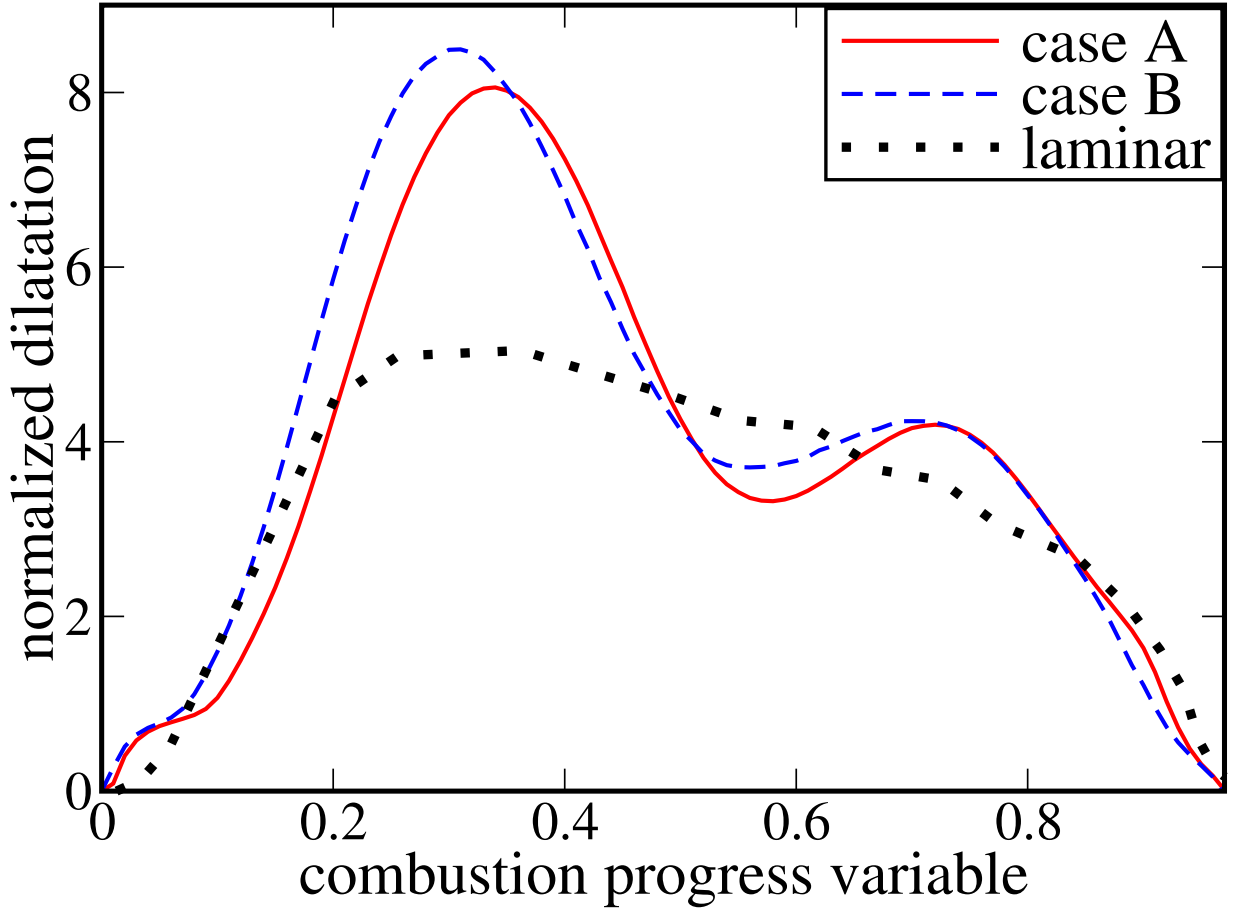
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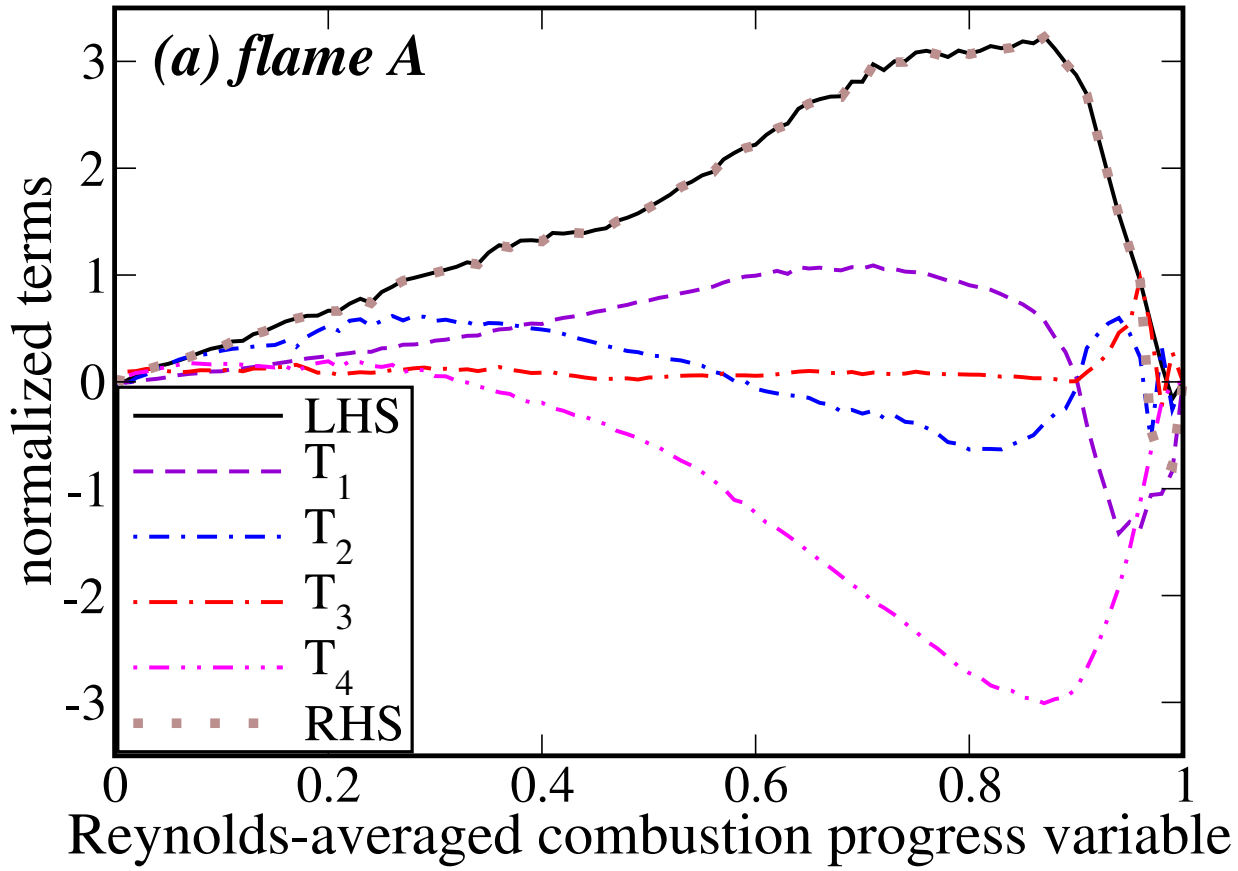
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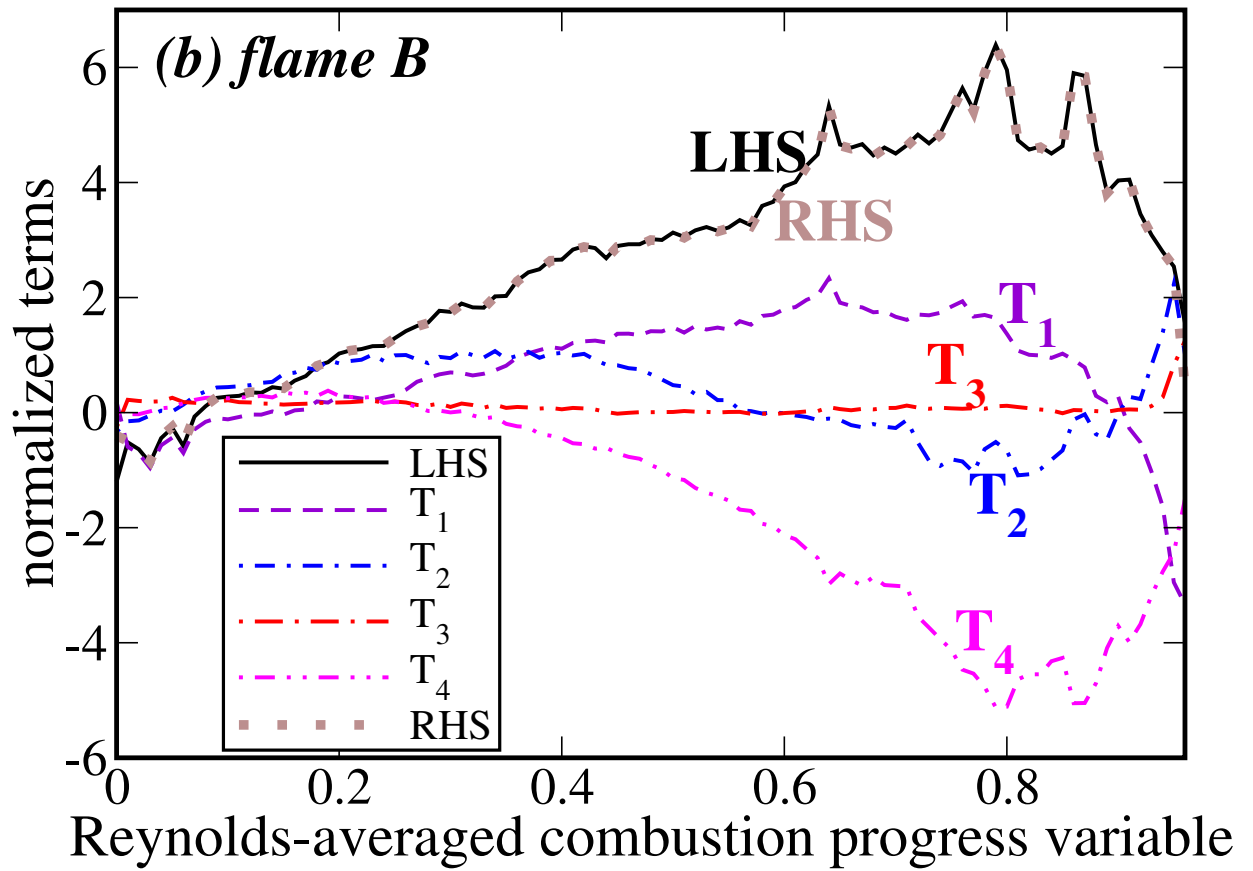
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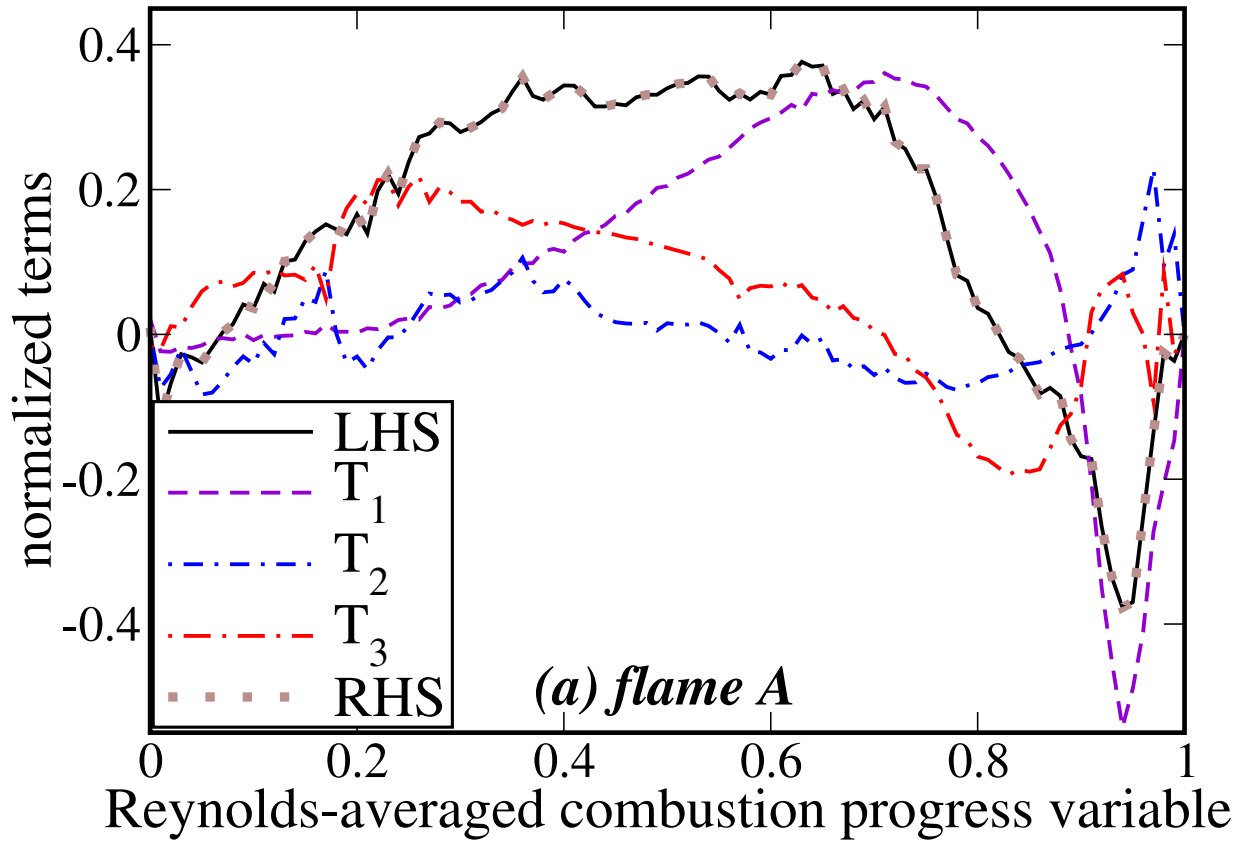
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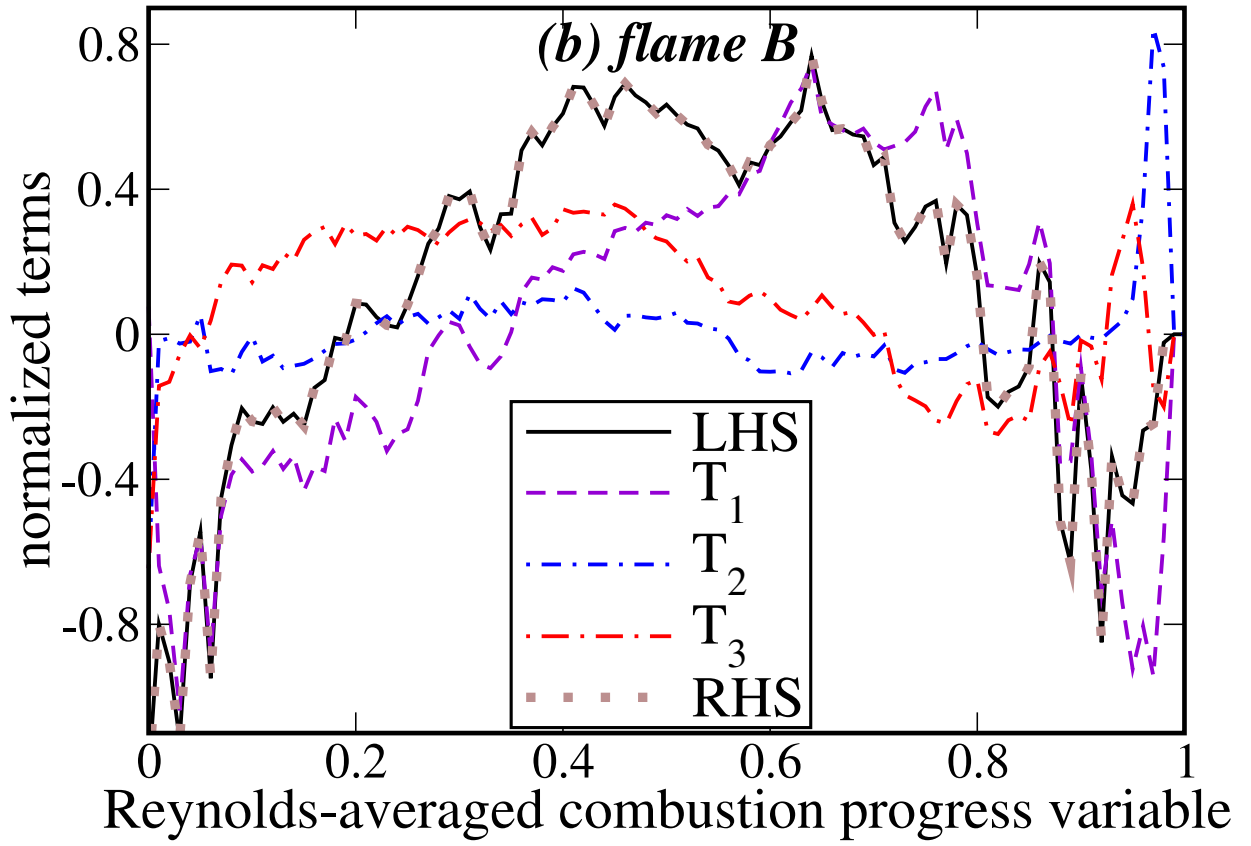
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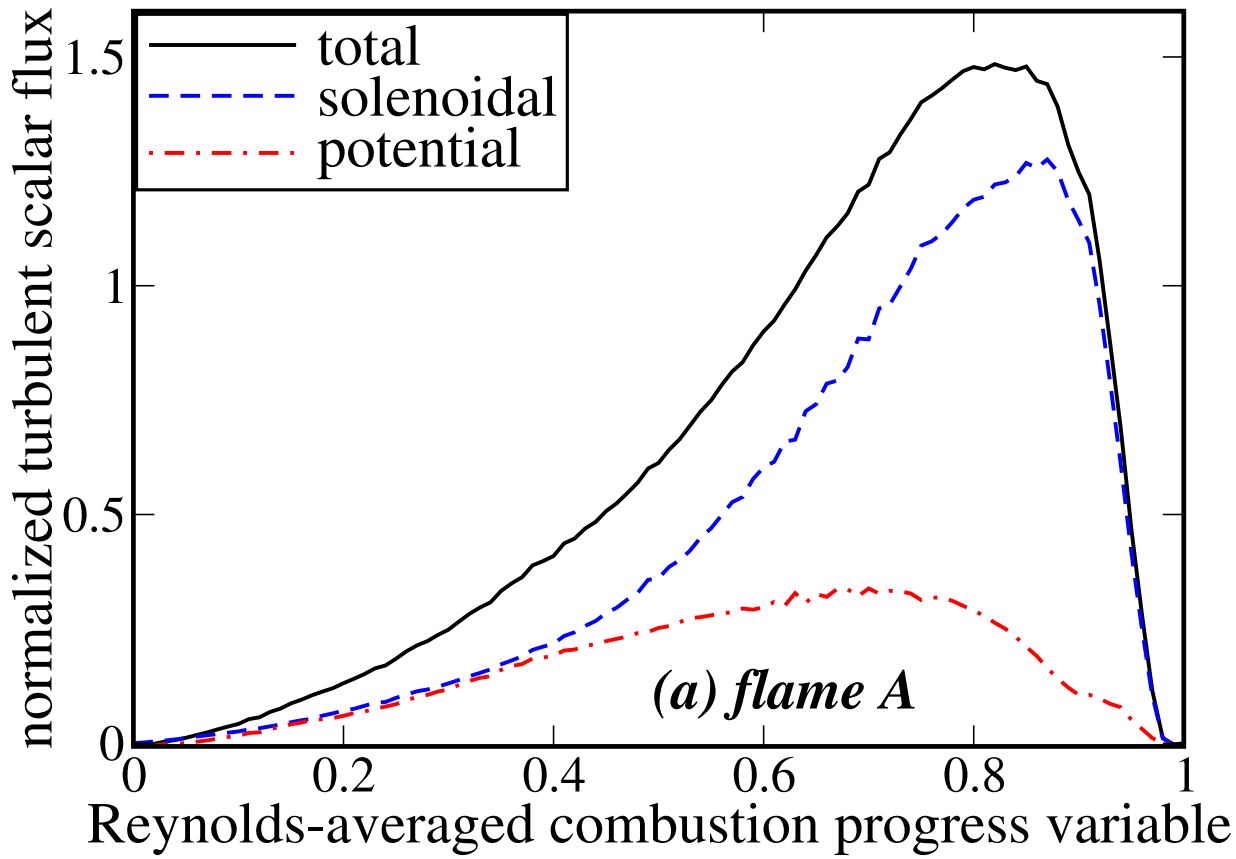
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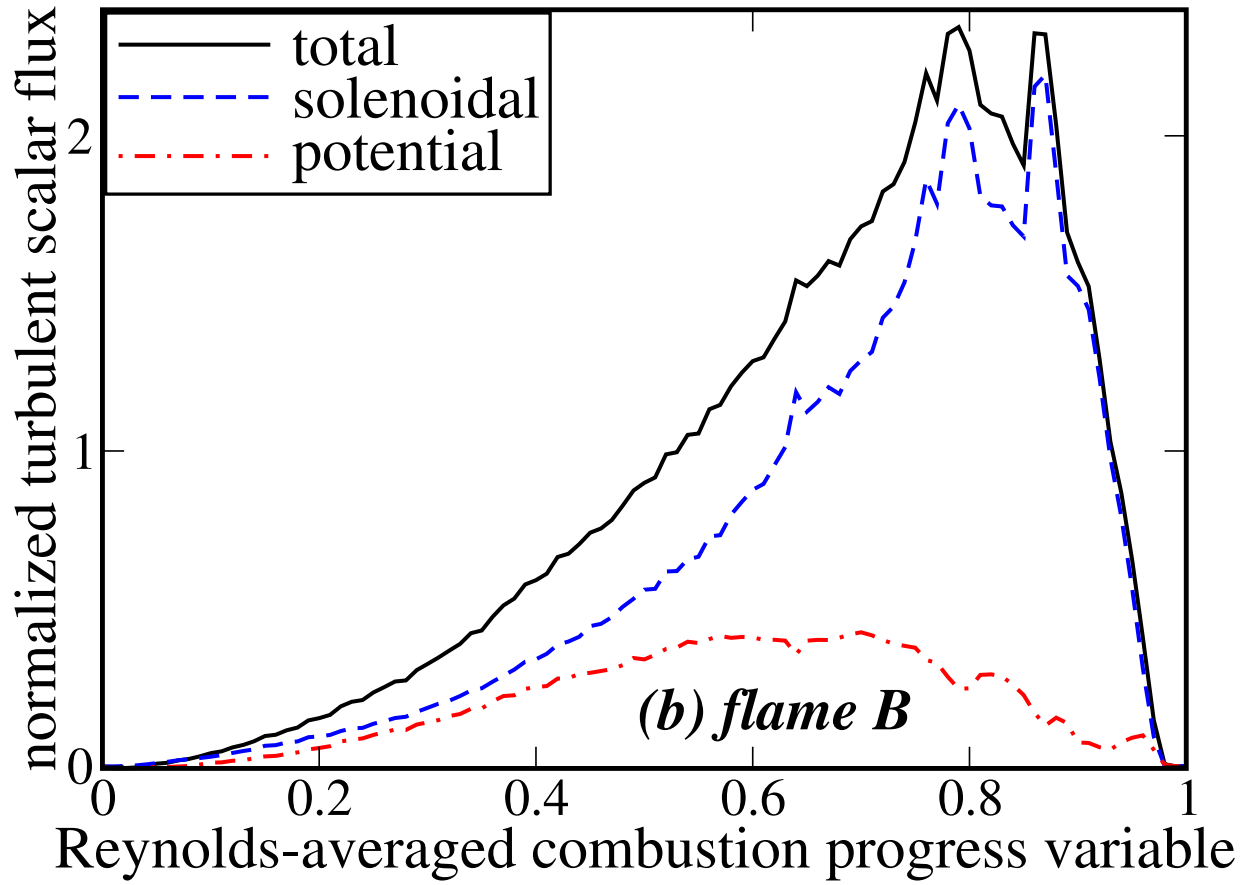
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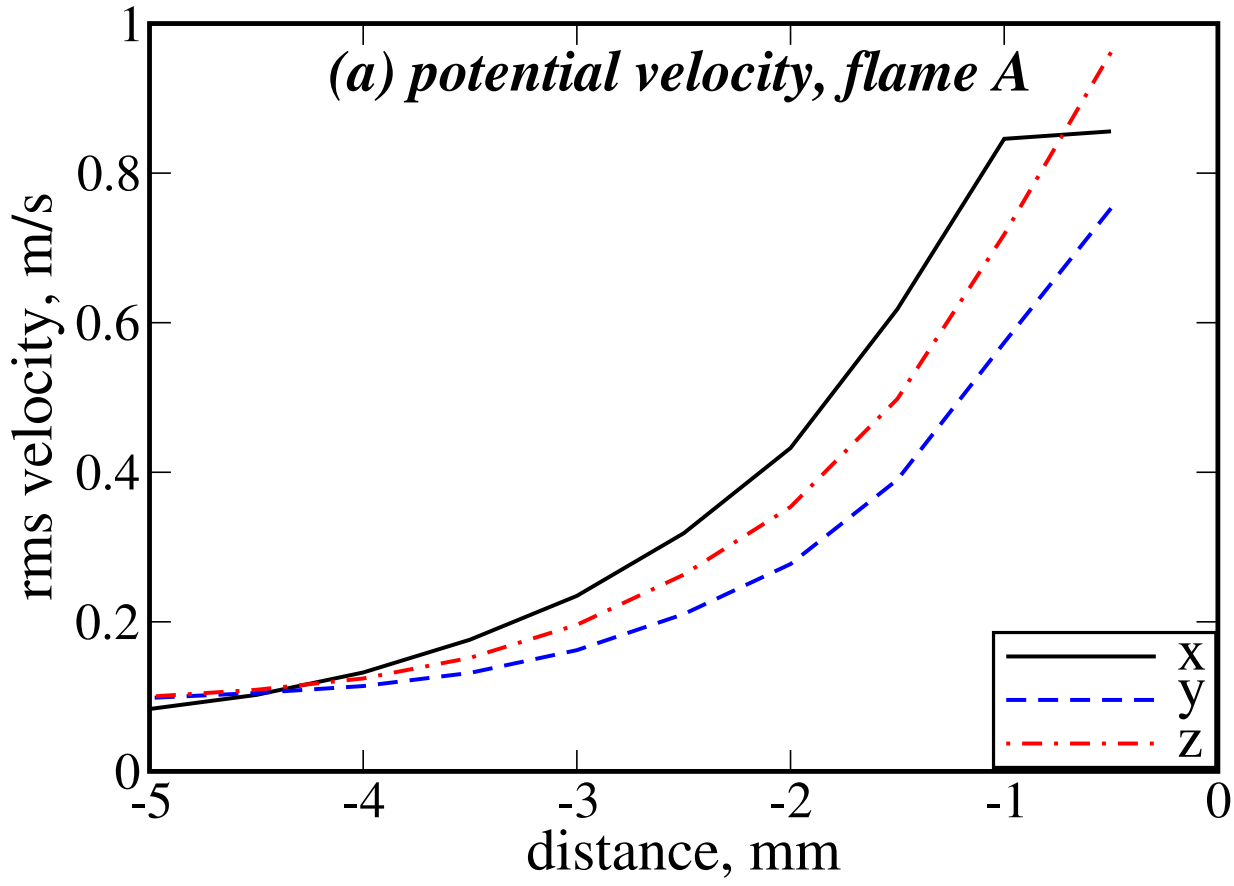
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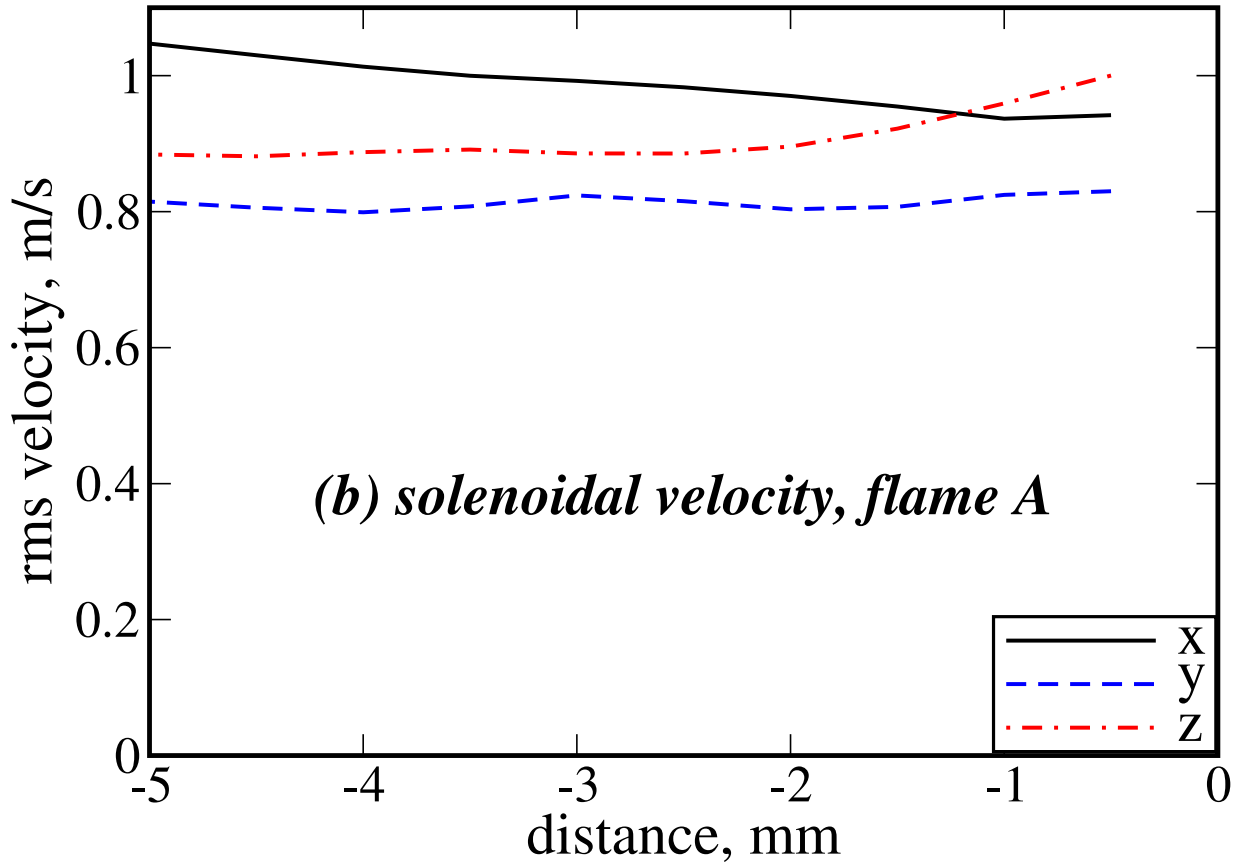
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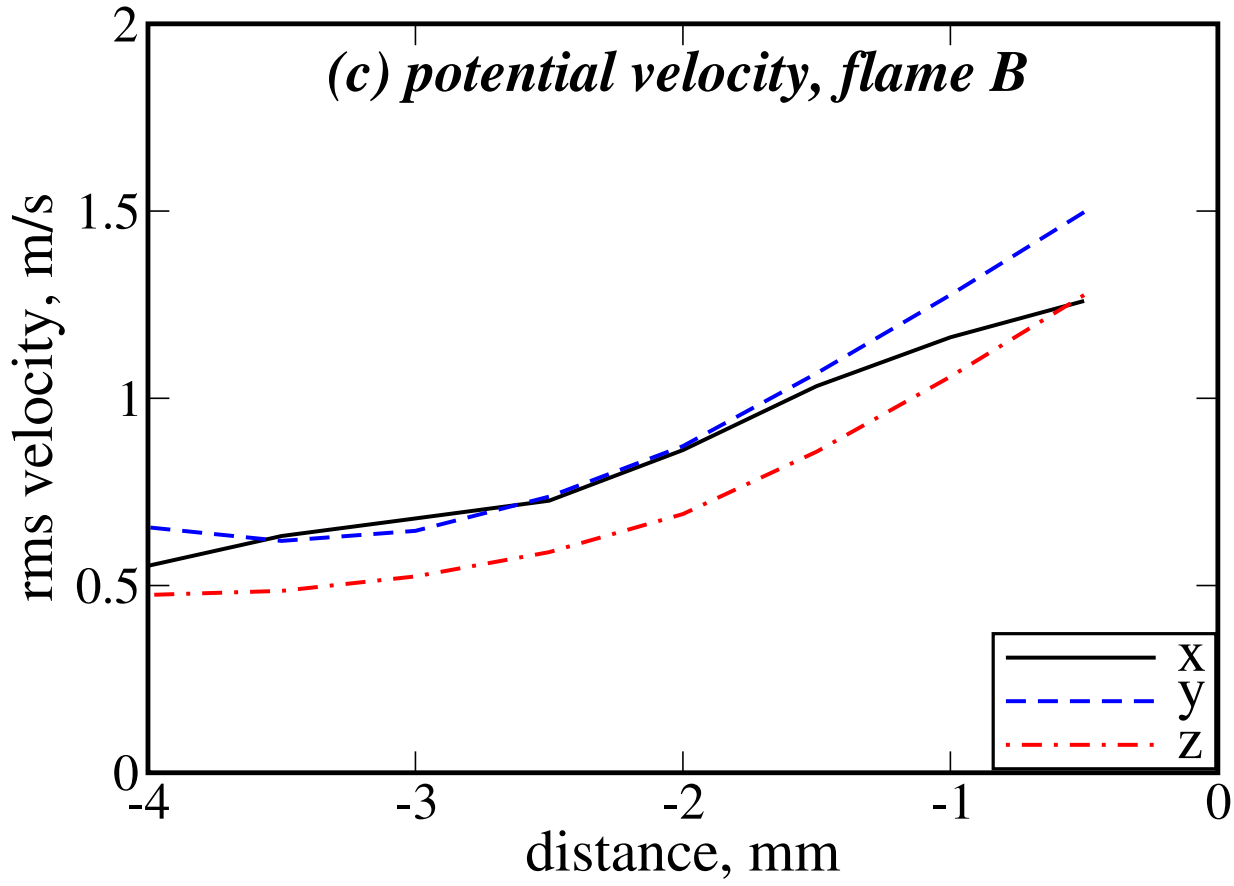
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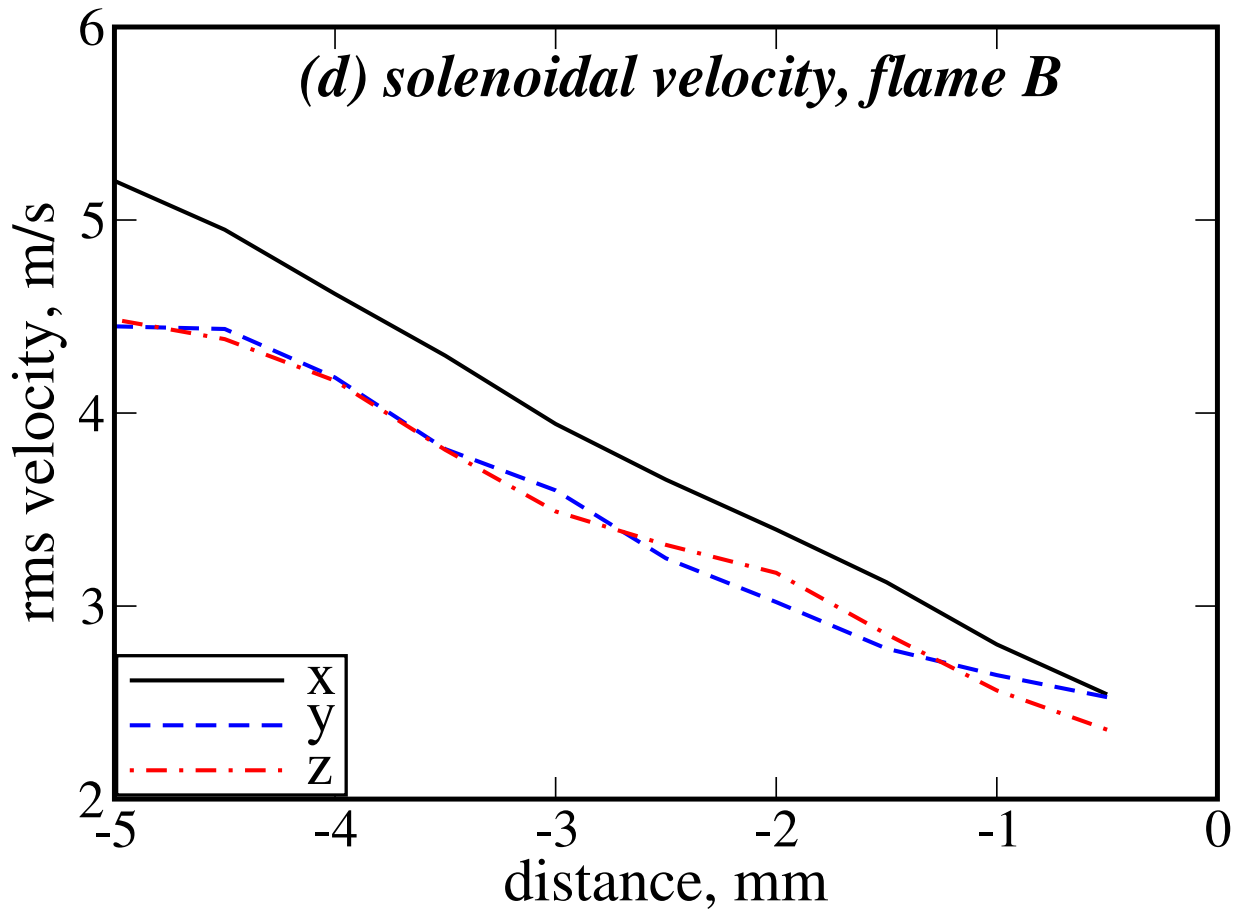
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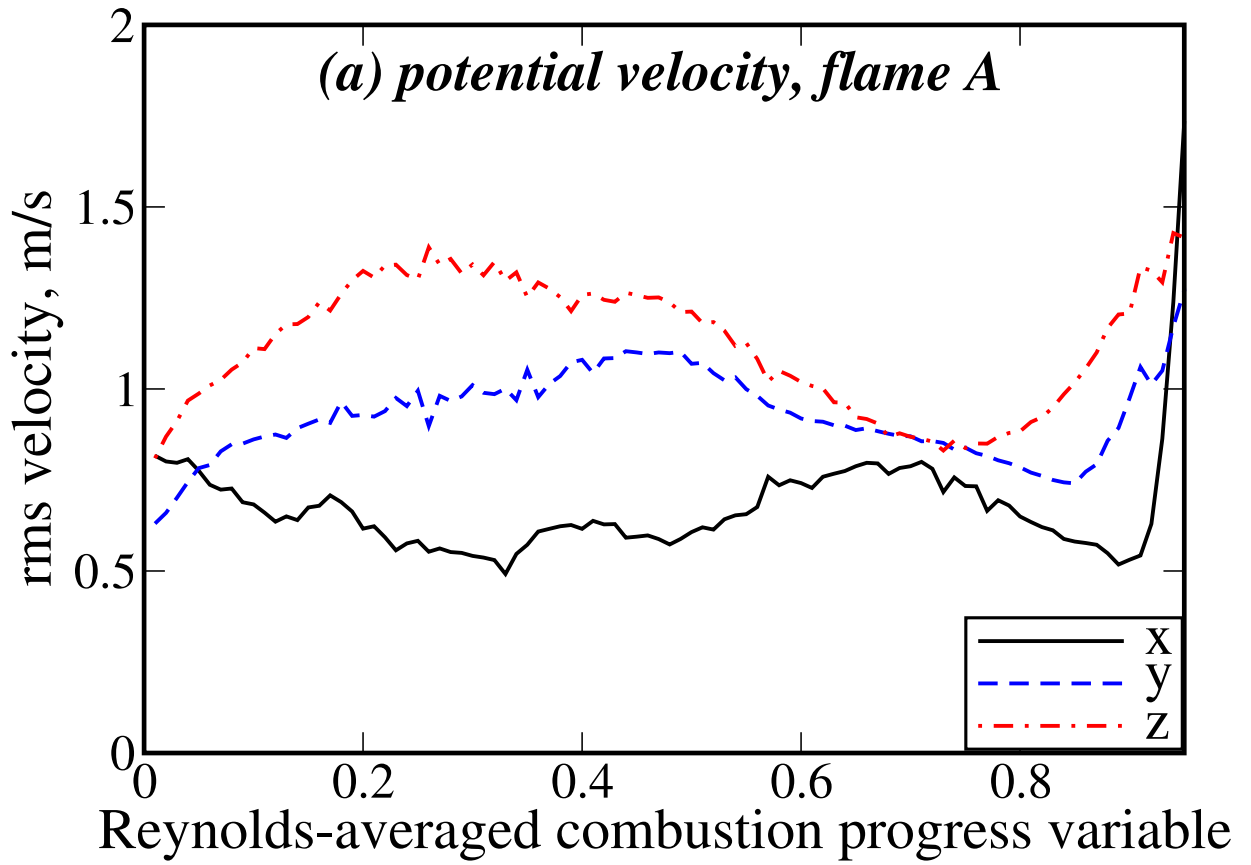
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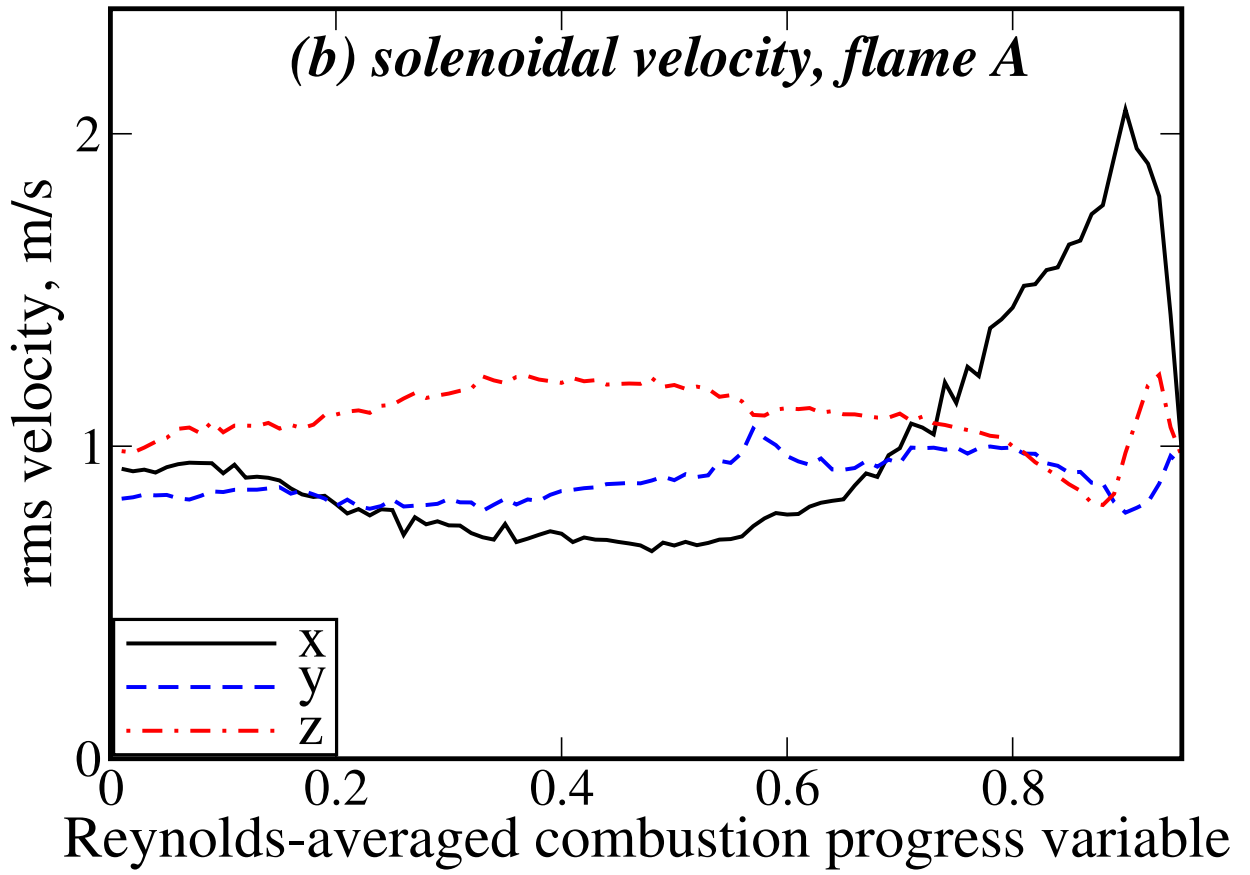


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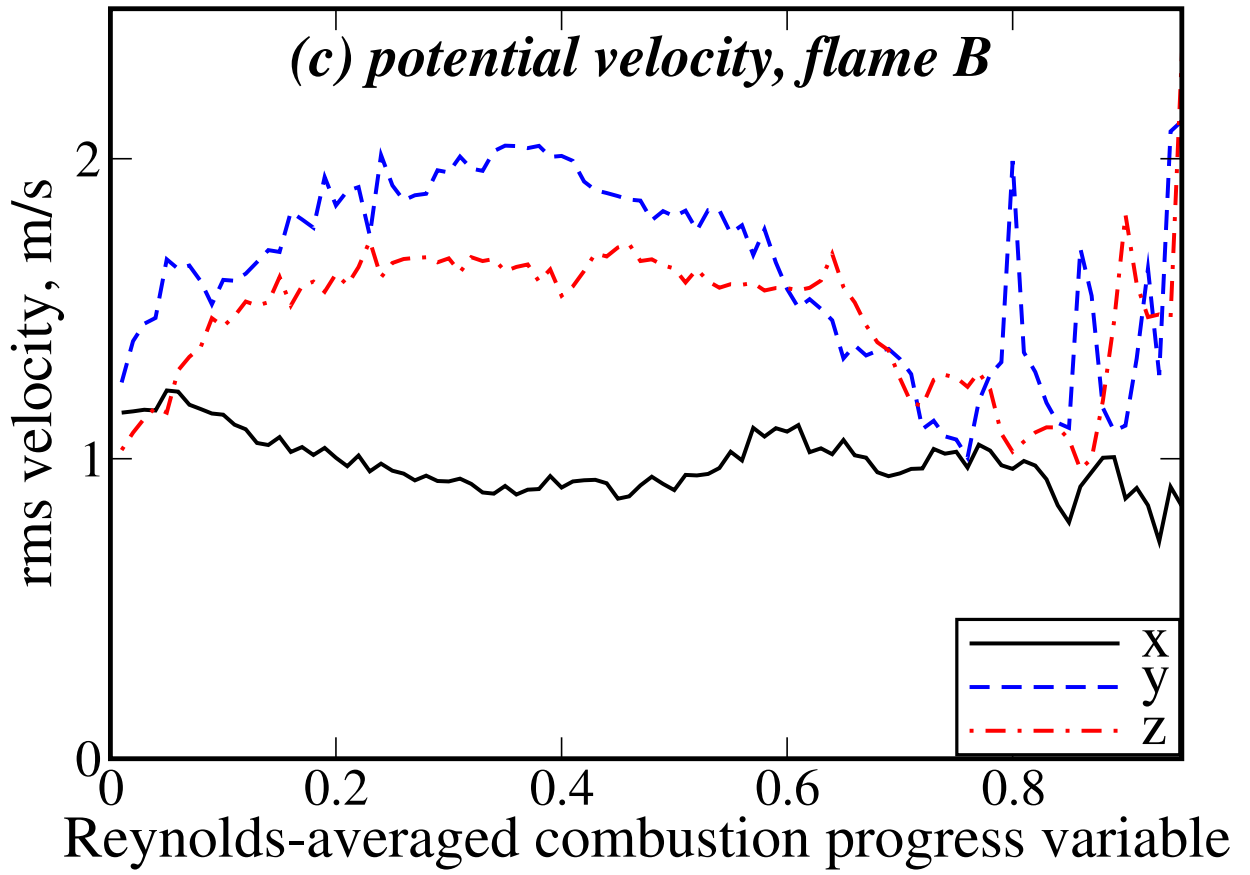
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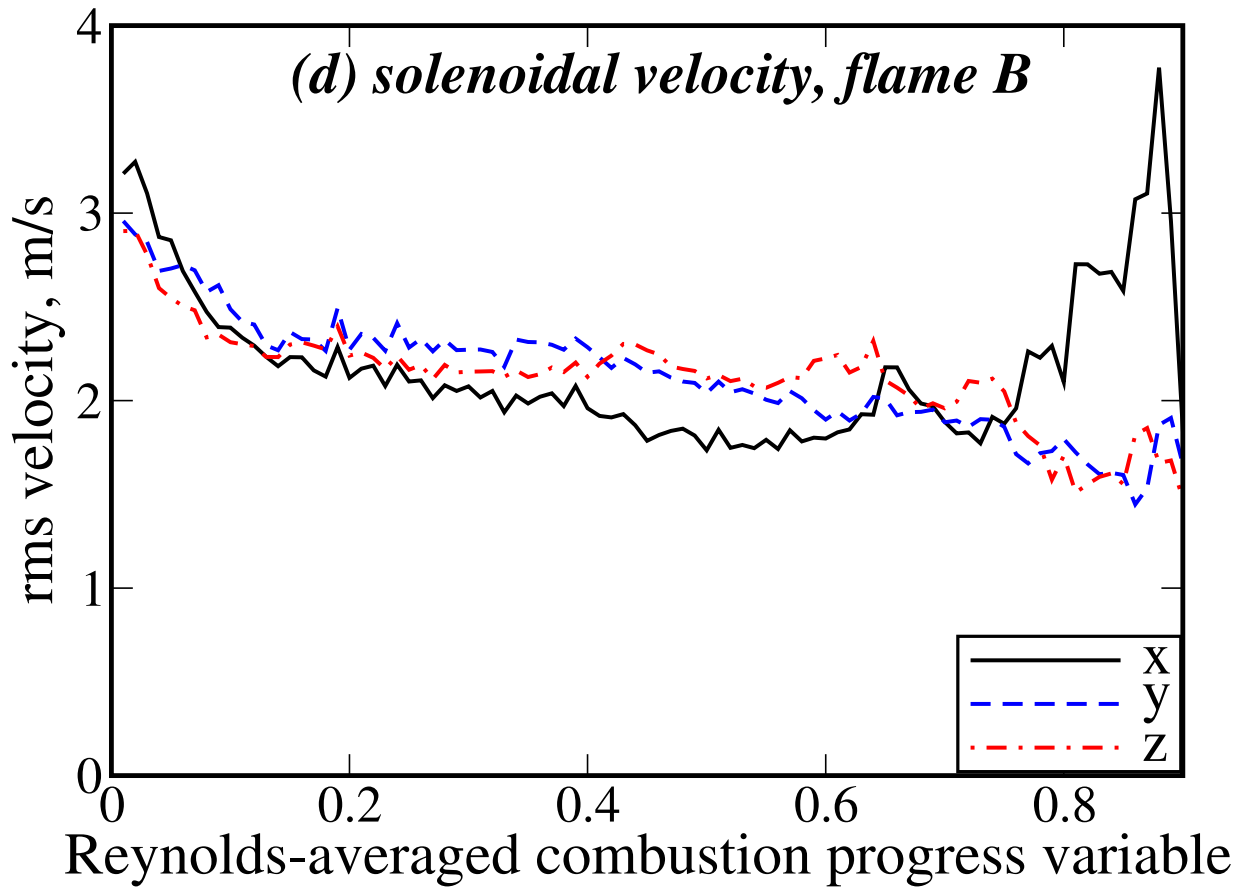


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