

Lagrangian Formulation of Turbulent Premixed Combustion

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The Lagrangian point of view is adopted to study turbulent premixed combustion. The evolution of the volume fraction of combustion products is established by the Reynolds transport theorem. It emerges that the burned-mass fraction is led by the turbulent particle motion, by the flame front velocity, and by the mean curvature of the flame front. A physical requirement connecting particle turbulent dispersion and flame front velocity is obtained from equating the expansion rates of the flame front progression and of the unburned particles spread. The resulting description compares favorably with experimental data. In the case of a zero-curvature flame, with a non-Markovian parabolic model for turbulent dispersion, the formulation yields the Zimont equation extended to all elapsed times and fully determined by turbulence characteristics. The exact solution of the extended Zimont equation is calculated and analyzed to bring out different regimes.

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Turbulent premixed combustion is a challenging scientific field involving nonequilibrium phenomena and playing the main role in important industrial issues such as energy production and engine design.

A Lagrangian point of view is here adopted, leading to a description of turbulent premixed combustion which takes into account, for all elapsed times, the turbulent dispersion, the volume consumption rate of reactants, and the flame mean curvature. The proposed approach generalizes and unifies classical literature approaches that are based on the so-called level-set method [1] or are based on the Zimont balance equation, originally hinted at by Prudnikov [3], also known as Turbulent Flame Closure model [2]. Moreover, the proposed formulation has the striking property to be compatible with every type of geometry and flow in an easier and more versatile way than previous approaches, and it emerges to be easily modifiable to include more detailed and correct physics. It is worth recalling that the Zimont equation was introduced on the basis of experimental observations and that a great effort has been undertaken to give a deeper theoretical foundation to it [2,4–6]. The present Lagrangian formulation constitutes a reliable theoretical support for the Zimont combustion model.

The process of turbulent premixed combustion is mainly characterized by flame propagation towards the unburned region and turbulent dispersion of the resultant product particles. The combustion process is described by a single dimensionless scalar observable, denoted as *average progress variable*, $0 \leq c(\mathbf{x}, t) \leq 1$, and representing the burned-mass fraction, i.e., the fraction of burned particles which are located in \mathbf{x} at time t . The value $c(\mathbf{x}, t) = 1$ describes the presence of only products and the value $c(\mathbf{x}, t) = 0$ describes the presence of only reactants. To avoid unnecessary mathematical difficulties, we consider a constant-density mixture and a zero-mean turbulent velocity field. Molecular diffusion is also neglected.

In this Letter, the fresh mixture is intended to be a population of particles in turbulent motion that, in a *statistical* sense, change from reactant to product when their average positions are hit by the flame. Let $\Omega(t)$ be the portion of space surrounded by the flame surface; then those particles with average position $\langle \mathbf{x} \rangle \in \Omega(t)$ are marked as burned particles. The occurrence in \mathbf{x} at time t of a particle transit is described by a probability density function (PDF). Let $p(\mathbf{x}; t|\mathbf{x}_0)$ be the PDF associated with a particle displacement where \mathbf{x}_0 is the initial condition of a Lagrangian trajectory and, without loss of generality, let $t = 0$ be the ignition instant. With the assumption that particle trajectories are not affected by the chemical transformation, the average progress variable $c(\mathbf{x}, t)$ turns out to be defined as the superposition of PDFs of burned particles, i.e., those $p(\mathbf{x}; t|\mathbf{x}_0)$ with $\langle \mathbf{x} \rangle \in \Omega(t)$. For a zero-average velocity field, the particle average position is $\langle \mathbf{x} \rangle = \mathbf{x}_0$ and then

$$c(\mathbf{x}, t) = \int_{\Omega(t)} p(\mathbf{x}; t|\mathbf{x}_0) d\mathbf{x}_0. \quad (1)$$

The evolution law for the progress variable $c(\mathbf{x}, t)$ is obtained applying Reynolds transport theorem to (1) which gives

$$\frac{\partial c}{\partial t} = \int_{\Omega(t)} \frac{\partial p}{\partial t} d\mathbf{x}_0 + \int_{\Omega(t)} \nabla_{\mathbf{x}_0} \cdot [\mathbf{u}(\mathbf{x}_0, t) p(\mathbf{x}; t|\mathbf{x}_0)] d\mathbf{x}_0, \quad (2)$$

where $\nabla_{\mathbf{x}_0}$ is the gradient with respect to \mathbf{x}_0 and $\mathbf{u}(\mathbf{x}, t)$ is the expansion velocity field of $\Omega(t)$.

Let the turbulent dispersion be represented by the general evolution equation

$$\frac{\partial p}{\partial t} = \mathcal{E}_{\mathbf{x}}[p], \quad p(\mathbf{x}; 0|\mathbf{x}_0) = \delta(\mathbf{x} - \mathbf{x}_0), \quad (3)$$

where the spatial operator $\mathcal{E}_{\mathbf{x}}[\cdot]$ includes the particle displacement statistics such as the variance $\sigma^2(t) = \langle \|\mathbf{x} - \mathbf{x}_0\|^2 \rangle / 3$.

Equation (2) is also governed by the volumetric expansion of $\Omega(t)$. This expansion is connected with the *consumption rate* that in a general form is set to be

$$\mathbf{u}(\mathbf{x}, t) = \mathcal{U}(\kappa, t)\hat{n}, \quad \hat{n} = -\frac{\nabla c}{\|\nabla c\|}, \quad (4)$$

where $\kappa(\mathbf{x}, t) = \nabla \cdot \hat{n}/2$ denotes the local mean *curvature*. Since molecular processes are neglected, the initial burning speed must be zero, i.e., $\mathcal{U}(\kappa, 0) = 0$. From (4) the location of the flame surface follows to be

$$\mathcal{L}_f(t) = \mathcal{L}_0 + \int_0^t \mathbf{u}(\mathcal{L}_f, \tau) d\tau. \quad (5)$$

Finally, inserting (3) and (4) in (2) gives

$$\begin{aligned} \frac{\partial c}{\partial t} = & \mathcal{E}_x[c] + \int_{\Omega(t)} \mathbf{u} \cdot \nabla_{\mathbf{x}_0} p d\mathbf{x}_0 + \int_{\Omega(t)} p \left\{ \frac{\partial \mathcal{U}}{\partial \kappa} \nabla_{\mathbf{x}_0} \kappa \cdot \hat{n} \right. \\ & \left. + 2\mathcal{U}(\kappa, t)\kappa(\mathbf{x}_0, t) \right\} d\mathbf{x}_0. \end{aligned} \quad (6)$$

The evolution of the progress variable is then led by three factors: turbulent motion, displacement speed of the contours of $c(\mathbf{x}, t)$ and their mean curvature. It is worth remarking that (6) cannot be reduced to the most widely used front propagation equations [7], and, since (6) follows from the exact Lagrangian definition (1), none of them is physically correct to model turbulent premixed combustion.

When particle motion is neglected, products and reactants turns out to be frozen, $\partial p/\partial t = 0$, so that $p \rightarrow \delta(\mathbf{x} - \mathbf{x}_0)$ and $\int_{\Omega(t)} \nabla_{\mathbf{x}_0} \cdot [\mathbf{u}(\mathbf{x}_0, t)p] d\mathbf{x}_0 = -\mathbf{u} \cdot \nabla c$. Here the identity $\nabla p = -\nabla_{\mathbf{x}_0} p$ has been used. In this limit case, using (4), Eq. (2) reduces to

$$\frac{\partial c}{\partial t} = \mathcal{U}(\kappa, t)\|\nabla c\|, \quad c(\mathbf{x}, t) = \begin{cases} 1, & \text{if } \mathbf{x} \in \Omega(t), \\ 0, & \text{otherwise,} \end{cases} \quad (7)$$

the celebrated Hamilton-Jacobi equation stated by Sethian [1] to track the flame front surrounding the burned volume $\Omega(t)$, which is related to the G -equation [8] and to the Kardar-Parisi-Zhang equation [9]. Equation (7) can be now interpreted as a consequence of Reynolds transport theorem.

When the normal \hat{n} to the contours of the progress variable is assumed constant, then the mean curvature κ is zero. Assuming an homogeneous, isotropic and stationary turbulence, for the Lagrangian PDF it holds $\nabla p = -\nabla_{\mathbf{x}_0} p$ and setting $\mathcal{U}(0, t) = \mathcal{U}(t)$ formula (6) turns out to be

$$\frac{\partial c}{\partial t} = \mathcal{E}_x[c] + \mathcal{U}(t)\|\nabla c\|. \quad (8)$$

It must be observed that in (8) the turbulent dispersion and the flame expansion enter in the progress variable evolution with the particle displacement variance $\sigma^2(t)$ and $\mathcal{U}(t)$, that are so far independent. However, in a proper combustion model they have to be mutually related since, when molecular processes are neglected, the flame front has to be solely fueled and carried by the turbulent dynamics of the reacting environment. To formulate a correspondence between particle spread and flame progression,

the expansion rate of the quadratic mean of particle displacement $r(\tau, t) = \sigma(t + \tau)/\sigma(t)$ is taken equal to the expansion rate of the flame front progression $\Delta_f(t) = \mathcal{L}_f(t) - \mathcal{L}_0$. In the mechanism here proposed, while the combustion evolves moving along the outward flame front normal, see Fig. 1, the expansion of σ is statistically related to the random oscillation of a particle moving forward and backward around its mean position. As a consequence, a *half* time step τ is necessary to the forward-moving flame front to have the *same* expansion rate than an unburned particle oscillating around its mean position: $r(\tau, t) = \Delta_f(t + \tau/2)/\Delta_f(t)$. Finally, noting that $r(0, t) = 1$ and performing the limit $\tau \rightarrow 0$, the joined process satisfies

$$\frac{1}{\mathcal{L}_f(t) - \mathcal{L}_0} \frac{d\mathcal{L}_f}{dt} = \frac{2}{\sigma(t)} \frac{d\sigma}{dt} = 2 \left. \frac{\partial r}{\partial \tau} \right|_{\tau=0}. \quad (9)$$

Let us introduce the function

$$\mathcal{D}(t) = \frac{1}{2} \frac{d\sigma^2}{dt} = \int_0^t B_L(\tau) d\tau, \quad (10)$$

where $B_L(t)$ is the Lagrangian velocity autocorrelation function. It is worth remarking that definition (10) is in agreement with the exact Taylor formula $\sigma^2(t) = 2 \int_0^t (t - \tau) B_L(\tau) d\tau$ that includes all turbulent dispersion regimes from the ballistic to the diffusive one passing through the inertial range. Using definitions (5) and (10) identity (9) can be written in terms of \mathcal{U} and \mathcal{D} and yields

$$\frac{\int_0^t \mathcal{U}(\xi) d\xi}{\mathcal{U}(t)} \frac{\mathcal{D}(t)}{\int_0^t \mathcal{D}(\xi) d\xi} = 1. \quad (11)$$

It follows that $\int_0^t [\mathcal{D}(t)\mathcal{U}(\xi) - \mathcal{U}(t)\mathcal{D}(\xi)] d\xi = 0$ for any $t \geq 0$. From the monotonicity of both \mathcal{U} and \mathcal{D} , since they are non-negative functions and $\mathcal{U}(0) = \mathcal{D}(0) = 0$, the following equality holds

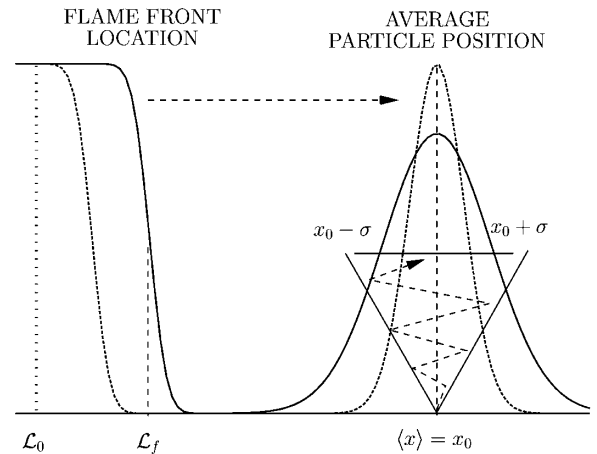


FIG. 1. Illustration of the forward motion of the flame front from the initial position \mathcal{L}_0 to $\mathcal{L}_f(t)$ and the expansion of the particle quadratic mean σ after a forward plus backward random walk around the average position $\langle x \rangle = x_0$.

$$\frac{\mathcal{D}(\xi)}{\mathcal{U}(\xi)} = \frac{\mathcal{D}(t)}{\mathcal{U}(t)}, \quad 0 \leq \xi \leq t, \quad (12)$$

so that, within the integration interval of ξ , the ratio $\mathcal{D}(\xi)/\mathcal{U}(\xi)$ must be constant. Moreover, for $t \rightarrow \infty$ both $\mathcal{D}(t)$ and $\mathcal{U}(t)$ are bounded, $\mathcal{D}(\infty) = \mathcal{D}_{\text{eq}}$ and $\mathcal{U}(\infty) = \mathcal{U}_{\text{eq}}$; therefore, such a constant is equal to

$$\frac{\mathcal{D}(t)}{\mathcal{U}(t)} = \frac{\mathcal{D}_{\text{eq}}}{\mathcal{U}_{\text{eq}}} = \lambda, \quad t \geq 0. \quad (13)$$

Identity (13) states that, by using definition (10), the whole evolution of the combustion process is *solely* established by $\sigma^2(t)$, and it constitutes a new result in literature [7]. Moreover, it determines not only the relation between the combustion drift and the background turbulent dispersion, but also the temporal evolution of the flame front location $\mathcal{L}_f(t)$ as it follows

$$\mathcal{L}_f(t) = \mathcal{L}_0 + \frac{\sigma^2(t)}{2\lambda}. \quad (14)$$

A similar result was already sketched by Biagioli [10] in the study of strongly swirled flows, but valid only for asymptotic long times. To validate the goodness of the physical argument that brought to expression (14), an experimental result discussed in the literature is used where σ and \mathcal{L}_f were simultaneously measured. The data come from Fig. 21 in Ref. [4] and they are attributed to unavailable measurements [11]. In the experimental setup, the gas mixture flows at the steady velocity $V = 26.0 \text{ ms}^{-1}$ and the data acquisition was performed at fixed distances $x[\text{mm}]$ from an origin. The measurement locations $x[\text{mm}]$ have been converted in elapsed times $t[\text{s}]$ by $t = x/V$ and \mathcal{L}_f and σ have been considered as measured in a reference frame in translation with the flow. Figure 2 shows the fit between the measurements of σ and Taylor formula, where the exponential autocorrelation function $B_L(t) = \langle u^2 \rangle \exp(-t/T_L)$ is assumed with $\mathcal{D}_{\text{eq}} = \langle u^2 \rangle T_L = 11 \times 10^3 \text{ mm}^2 \text{ s}^{-1}$ and $T_L = 2 \times 10^{-3} \text{ s}$. Here $T_L = \langle u^2 \rangle^{-1} \int_0^t B_L(\tau) d\tau$ denotes the Lagrangian integral timescale. Substituting the resulting analytic σ^2 in Eq. (14), the flame front position \mathcal{L}_f is correctly predicted. The experiment was performed twice with the same turbulence characteristics but with two different equivalence ratios F (that is the ratio of the fuel-to-oxidizer ratio to the stoichiometric fuel-to-oxidizer ratio): $F = 0.68$ and $F = 0.56$.

Let us consider now the simple non-Markovian parabolic model: $\mathcal{E}_x[p] \equiv \mathcal{D}(t)\nabla^2 p$. Equation (8) becomes the extension to all elapsed times of the familiar Zimont equation [2], which was historically formulated in the asymptotic regime $t \gg T_L$ with $\mathcal{D}(t)$ tending to \mathcal{D}_{eq} and $\mathcal{U}(t)$ to \mathcal{U}_{eq} . A critical review about it can be found in [4,6].

Despite the restriction $\kappa = 0$, other extensions of (8) to the initial regime $t < T_L$ are currently applied in engineering applications to study transient and geometrical effects

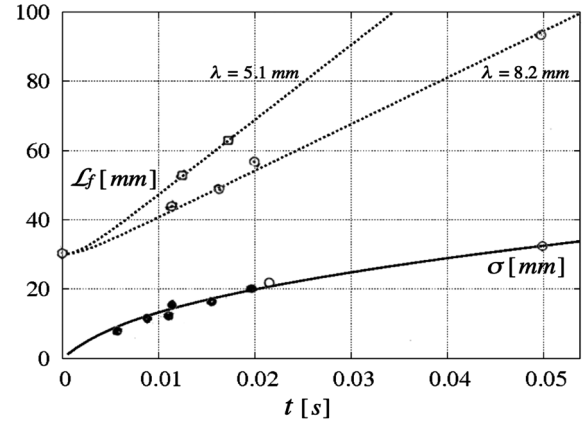


FIG. 2. Experimental validation of the propagation law (14). Lines are the plots of the analytic σ and the predicted flame front positions \mathcal{L}_f . The values $\lambda = 5.1 \text{ mm}$ and $\lambda = 8.2 \text{ mm}$ correspond to two different equivalence ratios $F = 0.68$ and $F = 0.56$, respectively.

in the developing phase of the flame [12] with practical fallouts in the design of spark-ignition engines [13].

With $\kappa = 0$, the study of Zimont equation is reduced to a one-dimensional problem along the normal direction to the flame front. The front speed (4) becomes $u(x, t) = -\mathcal{U}(t)\text{sgn}(\partial c/\partial x)$. Let the portion of space surrounded by the flame be $\Omega(t) = [\mathcal{L}_L(t), \mathcal{L}_R(t)]$, where \mathcal{L}_L and \mathcal{L}_R are the flame front positions defined in (5) on the left and on the right of the ignition point, respectively. Then the exact solution is

$$c(x, t) = \frac{1}{2} \left\{ \text{Erfc} \left[\frac{x - \mathcal{L}_R(t)}{\sqrt{2}\sigma(t)} \right] - \text{Erfc} \left[\frac{x - \mathcal{L}_L(t)}{\sqrt{2}\sigma(t)} \right] \right\}. \quad (15)$$

By setting $x = z - z_0$ and $\mathcal{L}_R(t) = z_f(t) - z_0$, in the limit $z_0 \rightarrow -\infty$ the progress variable becomes $c(z, t) = \text{Erfc}[(z - z_f(t))/(\sqrt{2}\sigma(t))]/2$, that is in agreement with several experimental results [4,6]. In particular, formula (14) can be plugged into solution (15) of the *extended* Zimont equation. With this model, now fully determined for all elapsed times by σ^2 , it is possible to perform a generally valid analysis on the flame *enhancement* and *quenching* and bring out the different regimes of the combustion process. The two examples of Fig. 3 display the evolution of $c(x, t)$ with the initial fully burned zone bounded by different flame front conditions: $\mathcal{L}_0 = \lambda/5$ and $\mathcal{L}_0 = 5\lambda$. For the plots, we have set $\langle u^2 \rangle = 1$, $T_L = 1$, $\lambda = 0.1$. Observe in Fig. 3(a) that, after the initial ignition instant, turbulent diffusion mixes together products and reactants so that the progress variable takes a bell-shape profile and in the central zone $c(x, t)$ is drained by the dispersion of the resulting product particles. If $c(\mathbf{x}, t)$ becomes less than a threshold value, quenching can be assumed. The larger is the ignition region the weaker is the draining, and, as illustrated in Fig. 3(b), no-draining occurs for an initial value \mathcal{L}_0 larger than a critical length scale \mathcal{L}_{0c} . The length scale \mathcal{L}_{0c} can be determined by the

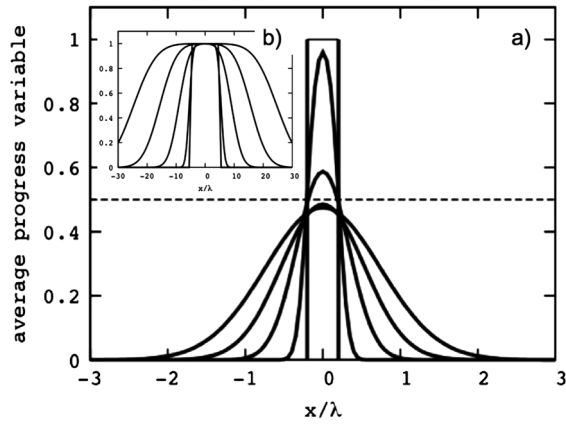


FIG. 3. Evolution of $c(x, t)$ starting from a fully burned zone: (a) $\mathcal{L}_0 = \lambda/5$ and $t = 0, 0.01T_L, 0.03T_L, 0.05T_L, 0.07T_L$; (b) $\mathcal{L}_0 = 5\lambda$ and $t = 0.01T_L, 0.1T_L, 0.3T_L, 0.5T_L, 0.7T_L$. In (a), the dashed line indicates the quenching threshold $c = 0.5$.

budget between the spread of the particle distribution, driven by $\mathcal{D}(t)$, and the expansion of $\Omega(t)$, driven by $\mathcal{U}(t)$. Introducing a pseudo diffusion coefficient for the combustion $\mathcal{U}(t)\mathcal{L}_0$, the budget emerges to be given by the ratio $\mathcal{U}(t)\mathcal{L}_0/\mathcal{D}(t) = \mathcal{L}_0/\lambda$. It emerges from this analysis that $\mathcal{L}_{0c} = \lambda = \mathcal{D}_{\text{eq}}/\mathcal{U}_{\text{eq}} = \sqrt{\mathcal{D}_{\text{eq}}\mathcal{T}}$, where $\mathcal{T} = \mathcal{D}_{\text{eq}}/\mathcal{U}_{\text{eq}}^2$ is a determination of the characteristic reaction time. When $\mathcal{L}_0 \ll \lambda$, the flame rapidly quenches after the initial ignition, see Fig. 3(a); when $\mathcal{L}_0 \gg \lambda$, the flame is immediately able to sustain itself, see Fig. 3(b), and the combustion propagates. This dependence on the size of \mathcal{L}_0 is the same as the one theoretically established for the Kolmogorov-Petrovskii-Piskunov models [14]. In the intermediate case $\mathcal{L}_0 \simeq \lambda$, when turbulence is not strong enough to drain $c(x, t)$ below the quenching threshold, $c(x, t)$, after an initial fall, is refilled and resustained by the combustion. This last behavior identifies the regime in which the process is dependent on the initial condition. Actually, considering the right semiaxis on the flame front location $x = \mathcal{L}_R(t)$, the two contributions of the Erfc functions in (15) become 1 and $\text{Erfc}\{\sqrt{2}[\mathcal{L}_0/\sigma + \sigma/(2\lambda)]\}$, respectively. Since $\sigma(t)$ is monotonic and increasing with $\sigma(0) = 0$, there exist two time scales τ_0 and τ_* defined by $\sigma(\tau_0) = \mathcal{L}_0$ and $\sigma(\tau_*) = 2\lambda$, respectively, which can be estimated from the scaling laws of $\sigma^2(t)$. For short times, $t \ll T_L$, when $\sigma^2 \simeq \langle u^2 \rangle t^2$, it turns out that $\tau_0 = \mathcal{L}_0/\langle u^2 \rangle^{1/2}$. After this transient regime which is dependent on the initial condition, the process tends asymptotically to be self-similar. The time scale τ_* turns out to be $\tau_* = 2(\langle u^2 \rangle/\mathcal{U}_{\text{eq}}^2)^{1/2}T_L$, if $\tau_* \ll T_L$, or $\tau_* = 2\lambda/\mathcal{U}_{\text{eq}}$, if $\tau_* \gg T_L$. This means that when $t < \tau_0 < \tau_*$ then $\mathcal{L}_0/\sigma > \sigma/(2\lambda)$ while when $t > \tau_*$ then $\mathcal{L}_0/\sigma < \sigma/(2\lambda)$. So when $t < \tau_*$ the second Erfc function is strongly variable, while when $t > \tau_*$ its argument begins to grow and the Erfc function tends rapidly to zero. Finally, when $t < \tau_*$ the average progress variable profile is not self-similar,

because each Erfc function in (15) has its own self-similarity variable, while for $t > \tau_*$ it is asymptotically self-similar with respect to the self-similarity variable $(x - \mathcal{L}_R(t))/\sigma(t)$. Then the time scale τ_* separates the initial not self-similar transient regime from the asymptotically self-similar regime. For long elapsed times, in the reference frame moving with the flame front, the smoothing effect of the turbulence spread decreases and asymptotically vanishes, making the profile of $c(x, t)$ steeper. The same arguments above can be applied to the left semiaxis. In addition, it is possible to expand the present formulation including the advecting mean velocity by following the same arguments formulated in [15] where \mathcal{D}_{eq} is changed in an effective diffusion coefficient with a nontrivial dependence on the mean velocity field. Then, by replacing (3) and (10) with a Lagrangian dispersion model for shear or cellular flow, the dependence of \mathcal{L}_{0c} on the mean velocity may be estimated as in [16,17].

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