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# Field equation for interface propagation in an unsteady homogeneous flow field

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The nonlinear scalar field equation governing the propagation of an unsteadily convected interface is used to derive a convenient expression for the average volume flux through such an interface in a homogeneous flow field. For a particular choice of the initial scalar field, the average volume flux through any such interface is expressed as a volume-averaged functional of the evolving scalar field, facilitating analysis based on renormalized perturbation theory and numerical simulation. It is noted that this process belongs to a different universality class from the propagation model of M. Kardar, G. Parisi, and Y.-C. Zhang [Phys. Rev. Lett. **56**, 889 (1986)].

A fundamental problem in combustion theory is the determination of the burning velocity of turbulent premixed flames in the laminar-flamelet regime, in which burned and unburned regions are separated by a thin, wrinkled interface.[1] This interface is convected by the unsteady flow field and propagates toward the unburned region at a normal velocity $u_F$ which depends on the local curvature of the interface as well as the local strain field. Furthermore, volumetric expansion due to heat release at the interface induces global as well as local distortions of the strain field.

As a paradigm of this and other processes involving the passage of a chemical reaction front through a stirred medium, the following simplified problem may be considered. A surface, initially planar, is convected by an unsteady homogeneous flow field, and the surface propagates relative to the flow field at a constant normal velocity $u_F$. This Huygens propagation mechanism is assumed to be passive in that it does not affect the fluid velocity field $\mathbf{v}(\mathbf{x},t)$. This velocity field may be regarded as a realization of Navier-Stokes turbulence, but this specification is not essential here.

Several fundamental issues concerning this as well as the more complicated processes of practical interest are as yet unresolved. Foremost among these is the issue of the existence of a steady-state turbulent burning velocity. The turbulent burning velocity $u_T$ is defined in this context as the volume flux through the evolving surface per unit cross-sectional (projected) area in the direction of propagation. It has not been established that, for a statistically steady flow field, the ensemble-average value of $u_T$ eventually converges to a constant. Furthermore, the dependence of $u_T$ on the rms velocity fluctuation $u'$ (a measure of turbulence intensity) and on Reynolds number is uncertain.

Resolution of these issues for Huygens propagation of a passive surface may provide insights relevant to the more complicated processes of practical interest. To investigate the simplified problem, it is useful to formulate the interface propagation problem as an initial value problem for a scalar field $G(\mathbf{x},t)$ whose level surfaces represent interfaces. An equation governing $G$ has been formulated,[2,3] and initial value problems have been solved numerically[3] for several configurations. Here it is shown that, for a particular choice of the initial scalar field, the average volume flux through a propagating interface convected by an unsteady homogeneous flow field can be expressed as a volume-averaged functional of the evolving scalar field. This formulation is advantageous for both computational and analytical study of the properties of $u_T$.

The field equation which we adopt is[2,3]

$$\frac{\partial G}{\partial t}+\mathbf{v}\cdot\nabla G=u_F|\nabla G| , \tag{1}$$

where $\mathbf{v}(\mathbf{x},t)$ is a given flow field. We briefly restate the derivation of this equation, which is a variant of a classical result.[4] The left-hand side of Eq. (1) is the convective derivative $DG/Dt$. It is easily seen that the source term on the right-hand side causes any level surface to propagate with a normal velocity $u_F$ relative to a local fluid element. For instance, consider some point $\mathbf{x}_0$ on any level surface $G=c$ at time $t_0$. In some neighborhood of $(\mathbf{x}_0,t_0)$, $G$ can be approximated by the lowest order terms in a Taylor expansion, namely,

$$G(\mathbf{x},t)=G(\mathbf{x}_0,t_0)+(\mathbf{x}-\mathbf{x}_0)\cdot\nabla G(\mathbf{x}_0,t_0)+(t-t_0)\frac{\partial G(\mathbf{x}_0,t_0)}{\partial t} . \tag{2}$$

In the limit $t\rightarrow t_0$, the point $\mathbf{x}(t)$ specified by

$$\frac{\mathbf{x}(t)-\mathbf{x}_0}{t-t_0}=\mathbf{v}(\mathbf{x}_0,t_0)-u_F\frac{\nabla G_0}{|\nabla G_0|} , \tag{3}$$

where $G_0\equiv G(\mathbf{x}_0,t_0)$, is on the level surface $G=c$ at time $t$. This follows from the definitions of $\mathbf{v}$ and $u_F$. Namely, a fluid element at point $\mathbf{x}_0$ is convected by the local fluid velocity $\mathbf{v}$, and the level surface propagates relative to the fluid element with velocity $u_F\mathbf{n}$, where $\mathbf{n}=-\nabla G_0/|\nabla G_0|$ is the unit vector normal to the level surface. (The convention is adopted that propagation is in the direction of decreasing $G$.) Therefore the right-hand side of Eq. (3) is the velocity of the level surface at $(\mathbf{x}_0,t_0)$, so $G(\mathbf{x},t)$

 

$=G(\mathbf{x}_0,t_0)$ to first order in $t-t_0$ for the above choice of $\mathbf{x}(t)$, as claimed. For this choice of $\mathbf{x}(t)$, Eq. (2) thus reduces to

$$\frac{\partial G_0}{\partial t}=-\frac{\mathbf{x}(t)-\mathbf{x}_0}{t-t_0}\cdot\nabla G_0 . \tag{4}$$

Substitution of Eq. (3) into Eq. (4) yields Eq. (1).

Although we have specified that $u_F$ is constant, this derivation is valid if $u_F(\mathbf{x},t)$ is taken to be any function of $G(\mathbf{x},t)$, $\mathbf{v}(\mathbf{x},t)$ and their derivatives. In particular, the aforementioned strain and curvature effects can be incorporated, as demonstrated below.

It is well known[3] that the solutions of initial value problems for Hamilton-Jacobi-type equations such as Eq. (1) develop discontinuities. In the present context, these discontinuities arise when portions of the propagating front converge on each other, thereby forming cusps. Generalized solutions which capture these features by means of limit processes can be defined, but such solutions are not unique. It has been shown[3] that the generalized solution which corresponds to the propagation process considered here is the so-called viscosity solution,[5,6] which is the unique solution obtained upon the addition of an infinitesimal diffusive term to the right-hand side of Eq. (1). It has also been shown[7] that a broad class of finite difference schemes for numerical solution of equations of this type yield controlled approximations to the viscosity solution. In particular, the numerical method adopted in the computations described shortly has this property. This point will be elaborated elsewhere.

In order to derive a convenient expression for $u_T$, we consider the time evolution of $G(\mathbf{x},t)$ viewed as an initial value problem, based on Eq. (1) and the initial condition $G(\mathbf{x},0)=x$, where the position vector $\mathbf{x}$ is expressed as $\mathbf{x}=(x,y,z)$. Since the field equation is nonlinear, the choice of initial condition is nontrivial. In particular, if the initial condition is transformed out of the problem by defining the alternative field $H(\mathbf{x},t)=G(\mathbf{x},t)-x$, for which $H(\mathbf{x},0)=0$, then substitution into Eq. (1) gives the field equation

$$\frac{\partial H}{\partial t}+\mathbf{v}\cdot\nabla H+\mathbf{i}\cdot\mathbf{v}=u_F(1+2\mathbf{i}\cdot\nabla H+\nabla H\cdot\nabla H)^{1/2} \tag{5}$$

for the new quantity $H$. (Here, $\mathbf{i}$ denotes the unit vector in the $x$ direction.) As discussed later, this is the most useful form of the initial value problem for analytical purposes. For now, we consider the initial value problem for the quantity $G$.

Initially, all level surfaces of $G$ are planes normal to $\mathbf{i}$. In the absence of convection, Eq. (1) indicates that any level surface $G=c$ remains planar with the same orientation, but moves with velocity $u_F$ in the $-\mathbf{i}$ direction. (Note that there is a length-scale normalization implicit in the initial condition.) Provided that mild regularity conditions are imposed on the fluctuating velocity field, overall propagation will also proceed in this direction in the presence of velocity fluctuations.

Taking $u_F$ to be constant and assuming that the flow field is homogeneous, we derive an expression for $u_T$ as follows. Consider a cylinder of infinitesimal cross-sectional area $dA=dy\,dz$ whose axis is parallel to $\mathbf{i}$. ($y$ and $z$ are the transverse coordinates.) For arbitrary $c$, we first seek an expression for the surface area $dS(c)$ of the portion of the level surface $G(\mathbf{x},t)=c$ which is contained within the cylinder. In terms of these quantities, $u_T$ can be expressed as

$$u_T=u_F\left\langle\frac{dS(c)}{dA}\right\rangle_{y,z} , \tag{6}$$

where the angle brackets denote an average over the transverse coordinates $(y,z)$ of the cylinder axis.

This specified subset of the level surface is not in general connected, reflecting the fact that a ray in the $x$ direction may intersect the surface more than once. (Most formulations of the propagation problem have difficulty treating surfaces which are multiply folded in this manner.) Each connected piece of this subset is treated as locally planar with unit normal vector $\mathbf{n}_j$ (again, adopting the convention that it points in the direction of decreasing $G$), where the index $j$ labels the pieces. The surface area of the $j$th piece is $dS_j=dA/|\mathbf{i}\cdot\mathbf{n}_j|$. Summing over $j$, we obtain

$$dS(c)=dA\sum_{j=1}^{J(c,y,z)}\frac{1}{|\mathbf{i}\cdot\mathbf{n}_j|} , \tag{7}$$

where the dependence of the number $J$ of such pieces on $c$ and on the transverse location of the cylinder axis is indicated explicitly. ($\mathbf{n}_j$ is likewise dependent on $c$, $y$, and $z$.)

Substituting Eq. (7) into Eq. (6), we express the transverse average as a normalized integral over the finite domain $y_1<y<y_2$, $z_1<z<z_2$, with the infinite-domain limit to be taken later. The result is

$$u_T(c)=\frac{u_F}{(y_2-y_1)(z_2-z_1)}\int_{z_1}^{z_2}\int_{y_1}^{y_2}\sum_{j=1}^{J(c,y,z)}\frac{1}{|\mathbf{i}\cdot\mathbf{n}_j|}dy\,dz , \tag{8}$$

where the argument of $u_T$ indicates that this expression for $u_T$ is based on a given, though arbitrary, value of $c$.

Though Eq. (8) is formally correct, a more useful expression is obtained by averaging over the parameter $c$, again by a normalized integration over a finite domain $c_1<c<c_2$, with the infinite-domain limit to be taken later. Substituting $\mathbf{n}=-\nabla G/|\nabla G|$, we obtain

$$u_T=\frac{u_F}{(c_2-c_1)(y_2-y_1)(z_2-z_1)}\int_{z_1}^{z_2}\int_{y_1}^{y_2}\int_{c_1}^{c_2}\sum_{j=1}^{J(c,y,z)}\frac{|\nabla G|_j}{|\mathbf{i}\cdot\nabla G|_j}dc\,dy\,dz , \tag{9}$$

where the index $j$ now denotes the $j$th intersection of a ray through $(y,z)$ in the $\mathbf{x}$ direction with the level surface $G=c$.

Equation (9) can be simplified by noting that the range of $c$ corresponds to all $x$ values for which $c_1<G<c_2$ along the aforementioned ray, and that each such $x$ value appears in the integrand exactly once. Therefore the integral over $c$ can be transformed into an integral over $x$. The Jacobian of the transformation is $dc/dx=|\mathbf{i}\cdot\nabla G|$, where the absolute value

appears because all ray increments $dx$ as well as all $dc$ increments make positive contributions to the total surface area. The Jacobian cancels the denominator of the integrand, giving

$$u_T=\frac{u_F}{(c_2-c_1)(y_2-y_1)(z_2-z_1)}\int_{z_1}^{z_2}\int_{y_1}^{y_2}\int_{c_1<G(x,y,z,t)<c_2}|\nabla G|\,dx\,dy\,dz\,. \tag{10}$$

For given $y$, $z$, and $t$, the range of the integral over $x$, specified implicitly by $c_1<G(x,y,z,t)<c_2$, is not connected in general, so evaluation of the finite-domain integral is not straightforward. However, the assumed homogeneity of the flow field simplifies the passage to an infinite domain. Namely, the statistics of the field $G-x$ are translationally invariant, so for $c_2-c_1$ much larger than the characteristic fluctuations of $G$ at given $x$, the range of $x$ in the integral may be approximated by $c_1<x<c_2$. Thus in the infinite-domain limit, the normalized integral in Eq. (10) reduces to the volume average of $|\nabla G|$. Note that the reduction to this simple result is a consequence of the assumed initial condition, $G(\mathbf{x},0)=x$.

If $u_F$ is allowed to depend on local properties, as discussed earlier, then the derivation is unchanged except that $u_F$ appears inside the sums and integrals rather than as a prefactor. Therefore the most general form of the result is

$$u_T=\langle u_F|\nabla G|\rangle\,, \tag{11}$$

where the angle brackets denote a volume average.

For analytical purposes, Eq. (5) for the field $H=G-x$ is the most useful field formulation because the $H$ field is homogeneous, with the simple initial condition $H(\mathbf{x},t)=0$. In terms of $H$, the expression for $u_T$ becomes

$$u_T=\langle u_F|\mathbf{i}+\nabla H|\rangle\,. \tag{12}$$

This expression for $u_T$ renders the field formulation tractable for analysis based on a stochastic representation of the velocity field, with the volume average interpreted as an ensemble average. Elsewhere, Yakhot[8] analyzes Eqs. (5) and (12) using methods of renormalized perturbation theory analogous to those previously[9] applied to a passively advected, diffusive scalar field. For Huygens propagation in homogeneous Navier-Stokes turbulence, he obtains a novel, closed form expression relating $u_T$ to $u_F$ and $u'$.

To illustrate the computational implementation of the field formulation, we have numerically solved the initial value problem for $G$ in a forced Navier-Stokes flow on a $32^3$ grid. In this calculation, $u_F$ was taken to be dependent on the local strain field and the local curvature of the level surface as prescribed by laminar-flame theory,[1] namely,

$$u_F=u_L(1-l_M\kappa)\,, \tag{13}$$

where $u_L$ represents the laminar flame speed in the absence of strain or curvature effects. The flame stretch $\kappa$ is given by

$$\kappa=-b+\nabla\cdot\mathbf{n}\,, \tag{14}$$

where $\mathbf{n}=-\nabla G/|\nabla G|$, $b=\mathbf{n}\cdot\mathbf{e}\cdot\mathbf{n}$, and $\mathbf{e}$ is the strain-rate tensor. The Markstein length $l_M$, whose value depends on flame chemistry, was taken to be $0.0125l_C$, where $l_C$ is the edge length of the computational domain. This choice of $l_M$ corresponds to a physically interesting case, as we will discuss elsewhere. We emphasize, however, that this illustrative computation should not be viewed as a fully realistic combustion simulation because thermal expansion is omitted.

The principal features of the flow field simulation are as follows. The kinematic viscosity is $0.002l_Cu_L$. To approximate a statistically steady flow field, the finite difference scheme used previously[10] was modified in this simulation to incorporate a constant energy constraint. This was implemented by means of a time-dependent low-wave number forcing applied to the strain field. The length scales in the flow field are established by the initial random selection of line vortices in each of three axis directions, with randomly selected core sizes. The core sizes are $\Delta$, $2\Delta$, and $4\Delta$, where $\Delta=l_C/32$, with populations of 512, 64, and 8, respectively. The circulation strength is set proportional to the $\frac{4}{3}$ power of the core size in order to mimic the cascade of turbulent energy. Although on this small mesh we do not expect to capture an inertial range in the energy spectrum, the simulation does reproduce attributes of the strain-rate tensor exhibited in Navier-Stokes simulations on larger grids.[11]

As noted earlier, an important unresolved question is

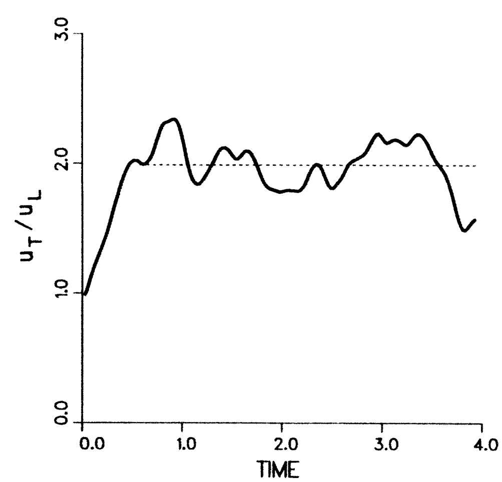


FIG. 1. Normalized volume flux $u_T/u_L$ through a level surface, estimated from a simulated realization of the field $G$, as a function of time expressed as a multiple of $l_I/u_L$. ($l_I$ is the turbulence integral scale and $u_L$ is the propagation velocity in the absence of strain or surface curvature.) $G$ was convected by a homogeneous Navier-Stokes velocity field with turbulence intensity $u'=1.2u_L$. The propagation velocity $u_F$ depends on strain and curvature effects as expressed by Eqs. (13) and (14). A time average over the period indicated by the dashed line yields $u_T/u_L=1.99$.

whether $u_T$ eventually converges to a constant value. Figure 1 shows a simulated time history of $u_T$, computed from the numerical solution for $G$ and the flow field using Eqs. (11), (13), and (14). The transition from an initial rise to fluctuations about a steady value is indicative of convergence to a constant ensemble-average value of $u_T$ in this case. For this realization, $u' = 1.2u_L$ and the integral length scale estimated from the transverse velocity correlation is $l_I \approx 0.1 l_C$. Therefore the characteristic time for large eddy turnover is $\tau = l_I/u' \approx 0.1 l_C/u_L$. This is consistent with the time scales for transient relaxation and subsequent fluctuations of $u_T$, as evident in Fig. 1.

Computations have been performed for other values of $u'$ and $l_M$, including $l_M = 0$ (corresponding to Huygens propagation), and similar features are observed. The plateau value of $u_T$ increases monotonically with $u'$ and decreases montonically with $l_M$. A quantitative parameter study, including additional details of the computations, will be presented elsewhere.

A practical advantage of the field formulation with Eq. (11) for $u_T$ is that the entire computational domain contributes to the estimate of $u_T$ at any epoch, in contrast to formulations in which a single interface within an Eulerian computational domain is simulated. Although the contributions of individual grid cells to the estimate are correlated, a substantial gain in overall computational efficiency is achieved. The gain is even greater when strain and curvature effects are incorporated, because the field formulation renders the computation of quantities governing these effects particularly convenient.

To place these results in perspective, we contrast the field formulation [e.g., Eqs. (5) and (12)], which is valid for propagation in any homogeneous velocity field irrespective of its dynamical origin, with the aforementioned analytical and numerical solution procedures, which have been applied specifically to propagation in hydrodynamic turbulence. Equation (5) can be regarded as a Langevin-type equation with a multiplicative vector noise term $\mathbf{v}(\mathbf{x},t)$ whose scaling properties determine the scaling properties of $u_T$. In this sense, Eq. (5) is analogous to the nonlinear Langevin equation for interface growth formulated by Kardar, Parisi, and Zhang.[12] They analyze the evolution of the height $h(y,z,t)$ of a growing interface which is restricted to be a single-valued function of the transverse coordinates $y$ and $z$ (a restriction not required in the present formulation). They obtain a source term of the form $u_F(1+\nabla h \cdot \nabla h)^{1/2}$, which resembles the right-hand side of Eq. (5). Their propagation model includes a linear diffusive term and an additive noise, rather than the multiplicative noise representing random convection. Renormalized perturbation analysis of their model predicts power-law growth of the interface zone with time. For the present formulation, computations (Fig. 1) and analysis (Ref. 8) indicate relaxation to statistically steady growth for at least one physically interesting specification of the fluctuating velocity field. Thus, the two formulations are not in the same universality class, indicating that propagation in a random convection field, as formulated here, constitutes a fundamentally distinct dynamical process.

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