QUASI-PROBABILITY APPROACH FOR MODELLING LOCAL EXTINCTION AND COUNTER-GRADIENT IN TURBULENT PREMIXED COMBUSTION

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Abstract
In opposition to standard probability distributions, quasi-probability distributions can have negative values which highlight nonclassical properties of the corresponding system. In quantum mechanics, such negative values allow for the description of the superposition of two quantum states. Here, we propose the same approach to model local extinction and counter-gradient in turbulent premixed combustion. In particular, the negative values of a quasi-probability correspond to the local reversibility of the progress variable, which means that a burned volume turns to be unburned and then the local extinction together with the counter-gradient interpretation follows. We derive the Michelson-Sivashinsky equation as the average of random fronts following the G-equation, and their fluctuations in position emerge to be distributed according to a quasi-probability distribution displaying the occurrence of local extinction and counter-gradient. The paper is an attempt to provide novel methods able to lead to new theoretical insights in combustion science.

Introduction
Turbulent premixed combustion requires a set of governing equations and a rich phenomenology follows. The set of governing equation includes: mass and momentum conservation, equation of state for gases, energy and species conservation. The nonlinearity of the problems requires closures and modelling. Self-extinction and counter-gradient are phenomena occurring in premixed combustion that require non-standard modelling approach or *ad hoc* modelling when standard approaches are adopted. Here we proceed with a research program presented in the last years at the Meetings of the Italian Section of the Combustion Institute [1,2,3]. The aim is to provide novel methods able to lead to new theoretical insights in combustion science. In particular, in the following we briefly report the derivation of the Michelson-Sivashinsky equation as the average of

random fronts following the G-equation [2,3], and we discuss that, since their fluctuations in position emerge to be distributed according to a quasi-probability distribution, then local extinction and counter-gradient are displayed by negative values of the quasi-probability emerging from such modelling approach. In the next section the main equations are derived, discussion and conclusion are reported in a further and ending section.

Statistical derivation of the Michelson-Sivashinsky equation
This section is based on [2,3] and it is here included for highlighting the role of the emerging quasi-probability into the proposed modelling approach.

Let the scalar function $G(x,t), x\in\mathbb{R}^n$, be a level surface that represents the front which splits the considered domain into burned and unburned sub-domains. Let x_c be a point on the level surface *G=c* at the instant t_0 . The level surface propagates with a consumption speed given by the laminar burning velocity s_L in the normal direction ***n*** relative to the mixture element and its evolution is described by the following Hamilton-Jacobi equation where the flow velocity field is ***u***

$$\frac{\partial G}{\partial t}+u\cdot\nabla G=s_L\|\nabla G\| \quad , \quad n=-\frac{\nabla G}{\|\nabla G\|} \quad . \tag{1}$$

Let the front motion be described by the random process $X_c^\omega(\hat{x},t)$ where ω labels any independent realization and the mean value of X_c^ω be denoted by $\langle X^\omega(\hat{x},t)\rangle=\hat{x}(t)$, then if $P_c(x_c;t|\hat{x})$ is the corresponding PDF, with initial condition $P_c(x_c;t_0|\hat{x})=\delta(x-x_0)$, the mean flame position is given by the integral

$$\langle x_c\rangle=\int_{\mathbb{R}^n} x_c P_c(x_c;t|\hat{x})\,d x_c=\hat{x}(t) \quad . \tag{2}$$

Introducing $\check{G}(\hat{x},t)$,with $\check{G}(\hat{x},t_0)=\check{G}(x_0,t_0)=c$, as the implicit formulation of the mean flame position $\hat{x}$, the ensemble averaging of (1) gives [5]

$$\frac{\partial \check{G}}{\partial t}+\hat{u}\cdot\nabla\check{G}=\widehat{s_L n}\cdot\nabla\check{G}. \tag{3}$$

Since the G-equation can be derived on the basis of considerations about symmetries, there is a unique model for the RHS term of equation (3) providing a relation between the laminar burning velocity s_L and the turbulent burning velocity s_T [5], i.e.

$$\widehat{s_L n} = s_T \check{n} \quad , \qquad \check{n} = -\frac{\nabla \check{G}}{\|\nabla \check{G}\|} s \quad . \tag{4}$$

Finally, combining equation (3) and (4), the *G*-equation that describes the surface motion along the mean flame position results to be

$$\frac{\partial \check{G}}{\partial t} + \hat{u} \cdot \nabla \check{G} = s_T \|\nabla \check{G}\| \quad . \tag{5}$$

The one-dimensional Michelson-Sivashinsky equation reads [6]

$$\frac{\partial g}{\partial t} = \frac{\partial^2 g}{\partial x^2} - \left(\frac{\partial g}{\partial x}\right)^2 - D_x^1 g \quad , \tag{10}$$

where D_x^1 is the fractional derivative of order 1 in the Riesz-Feller sense with Fourier symbol $-|\xi|$, which differs from the classical first derivative, and it is related to the Hilbert transform by the formula

$$D_x^1 g = \frac{1}{\pi} \frac{d}{dx} \int_{-\infty}^{+\infty} \frac{g(x')}{(x' - x)} dx' . \tag{11}$$

Let us introduce the field $g(x,t)$ in analogy with [7], i.e.,

$$g(\mathrm{x,t}) = \int \check{G}(\hat{x}, \mathrm{t}) P_c(x - \hat{x}, \mathrm{t}) \mathrm{d}\hat{x} . \tag{12}$$

It is well-known that the dispersion relation of equation (10) is

$$e^{-\xi^2 t + |\xi| t} . \tag{13}$$

This suggests the following fractional differential equation for the PDF of the fluctuations of the front position:

$$\frac{\partial P_C}{\partial t} = \Delta \mathrm{P}_C + (-\Delta)^{1/2} P_C, \quad P_C(x,0) = \delta(x) . \tag{14}$$

Actually, the dispersion relation (13) is the Fourier transform of the Green function of (14). It is here highlighted that the PDF of fluctuations which solves (14) emerges to be a quasi-probability distribution showing negative values that requires high care, see Figure.

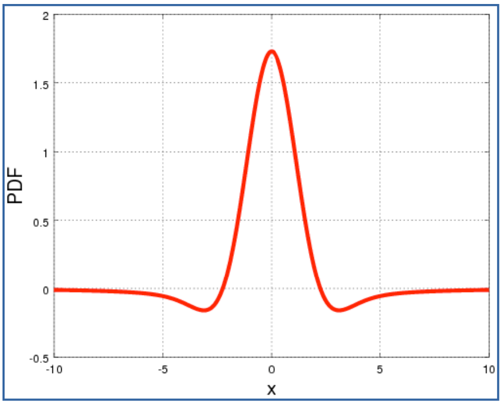

Figure: Quasi-probability distribution solution of (14).

The evolution equation of the function $g(x,t)$ results to be:

$$\frac{\partial g}{\partial t}=\frac{\partial^2 g}{\partial x^2}-D_x^1 \mathrm{g}+\int s_T(\hat{x},\mathrm{t})P_C(x-\hat{x},\mathrm{t})\,\mathrm{d}\hat{x}. \quad (15)$$

Comparing (10) and (15) we have

$$-\left(\frac{\partial g}{\partial x}\right)^2=\int s_T(\hat{x}\,\mathrm{t})P_C(x-\hat{x},\mathrm{t})\,\mathrm{d}\hat{x}\equiv\omega, \quad (16)$$

that in Fourier domain reads

$$\tilde{\omega}=\tilde{s}_T\tilde{P}_c=\tilde{s}_T\exp\left(-\xi^2 t+|\xi|t\right)\quad , \quad (17)$$

and the turbulent burning velocity turns out to be

$$s_T(x,t)=\frac{1}{2\pi}\int\exp(-i\xi x)\exp\left(\xi^2 t-|\xi|t\right)\tilde{\omega}(\xi,t)\,d\xi\quad . \quad (18)$$

Discussion and conclusion

In the previous section we showed that when the Michelson-Sivashinsky equation is derived as the ensemble average of random fronts governed by the G-equation, then the spatial fluctuations of the positions of the random fronts are distributed accordingly to a quasi-probability. Quasi-probability distributions display negative values, see Figure, that require high care in their interpretation. In particular, by using Fourier inverse transformation, the quasi-probability that solves (14) can be written in the following integral form

$$P_c(x,t)=\frac{1}{2\pi}\int \exp(-i\xi x)\exp(-\xi^2 t+|\xi|t)\,d\xi, \tag{19}$$

such that it results to be close to the representation of the Wigner quasi-distribution for quantum optics.

The negative values highlight where statistically the fraction of burned mixture is replaced by unburned mixture. In fact, if we integrate (12) in space we have that in correspondence of the negative values of the quasi-probability there is a reduction of the mass amount. The propagation of the front is slowed. For this reason, we propose that these negative values can be interpreted as due to local extinction and counter-gradient phenomena. Local reversibility of the value of the progress variable occurs because of the entering of fresh mixture into a volume just now fully burned. This effect can be ascribed first to the local extinction, that stops the propagation of the combustion, and then to the so-called counter-gradient, which is generated by the density difference between reactants and products, that pushes back the front of the burned mixture.

In formulae, this interpretation can be stated as follows. Let $C=|C|e^{iQ}=C_R+iC_I$ be the progress variable with real and imaginary part. Then it holds $C_R^2=|C|^2-C_I^2$, and if the $g(x,t)$ defined in (12) corresponds to the real part, i.e. $g=C_R$, then we have

$$g=|C|+F(C_I), \tag{20}$$

where

$$|C|=\int_{P_c>0}\check{G}(\hat{x},\mathrm{t})P_c(x-\hat{x},\mathrm{t})\,\mathrm{d}\hat{x}, \tag{21}$$

$$F(C_I)=\int_{P_c<0}\check{G}(\hat{x},\mathrm{t})P_c(x-\hat{x},\mathrm{t})\,\mathrm{d}\hat{x}<0. \tag{22}$$

The imaginary part results to be

$$C_I=e^{i(Q-\pi/2)}\int_{P_c>0}\check{G}(\hat{x},\mathrm{t})P_c(x-\hat{x},\mathrm{t})\,\mathrm{d}\hat{x}+i\int\check{G}(\hat{x},\mathrm{t})P_c(x-\hat{x},\mathrm{t})\,\mathrm{d}\hat{x}. \tag{23}$$

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