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LETTER TO THE EDITOR

Upper bounds for the reaction front in *d*-dimensional turbulent flow

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Abstract. We develop an asymptotic method that yields analytic results for the upper bounds for the ensemble averaged reaction front position and speed in a *d-dimensional* high Reynolds number turbulent flow. The chemical reaction is assumed to be of Kolmogorov–Petrovskii–Piskunov type and the velocity is an incompressible Gaussian random field. In addition to the general formalism, some examples are worked out in detail.

The study of the propagation of the reaction front in a random environment is of importance in a variety of problems in physics and chemistry [1–8]. The most widely studied quantity in such problems is the average rate at which the reaction front propagates throughout the random medium. In recent papers [6, 7] we considered the problem of the propagation of the chemical front by using the Kolmogorov–Petrovskii–Piskunov equation with the random convection term involving simple shear flow with a power energy spectrum and infrared divergence (see also [3, 4, 8]). In particular, we found that the propagation rate is very sensitive to the detailed structure of random flow. Hence it is desirable to extend these results by considering a more realistic model for the random velocity field and develop the general formalism for obtaining the propagation rate in the long-time, large-distance limit.

In this letter we shall present a new approach to the calculation of an upper bound for the ensemble averaged reaction front position and speed for general dimensionality. The main mathematical tool is a functional integral technique based on stochastic differential equations [9–10].

The problem of reaction front propagation can be formulated in terms of the modified Kolmogorov–Petrovskii–Piskunov (KPP) equation for a dimensionless scalar field $\varphi(t, \boldsymbol{x})$ [3, 4, 6, 7]:

$$\frac{\partial \varphi}{\partial t} + \boldsymbol{v}(t, \boldsymbol{x}) \cdot \nabla \varphi = D\nabla^2 \varphi + c(\epsilon \boldsymbol{x}, \varphi)\varphi \qquad \boldsymbol{x} \in \mathbb{R}^d \tag{1}$$

where the nonlinear term $c(\varphi)\varphi$ describing the reaction rate is assumed to be of Kolmogorov–Petrovskii–Piskunov type, i.e.

$$c(\epsilon \boldsymbol{x}, 0) = \max_{\varphi \in [0,1]} c(\epsilon \boldsymbol{x}, \varphi) > 0 \qquad c(\epsilon \boldsymbol{x}, 1) = 0 \tag{2}$$

and the random velocity $\boldsymbol{v}(t, \boldsymbol{x})$ is a Gaussian solenoidal field with zero mean and correlation tensor

$$\langle v_i(t, \boldsymbol{x}) v_j(\tau, \boldsymbol{y}) \rangle = B_{ij}(t - \tau; \boldsymbol{x}, \boldsymbol{y}). \tag{3}$$

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Here and in what follows the angular brackets $\langle\cdot\rangle$ denote ensemble averaging over the velocity statistics. The space and time variables are measured in units of the dissipation length and time scales [6, 7].

The initial condition is

$$\varphi(0, \boldsymbol{x}) = \varphi_0(\epsilon \boldsymbol{x}) \tag{4}$$

where the initial distribution $\varphi_0(\epsilon \boldsymbol{x})$ is assumed to be a positive, bounded function that varies on the integral scale of turbulence and has the support

$$\Omega = \left\{ \boldsymbol{x} \in \mathbb{R}^d : \varphi_0 > 0 \right\}.$$

It is also assumed that the support Ω does not coincide with $\mathbb{R}^d$.

The initial value problem, equations (1)–(4), involves a small parameter $\epsilon = Re^{-3/4}$, the ratio of the Kolmogorov length scale η to the integral length scale l_0; Re is a Reynolds number. This small parameter allows us to separate the problems of determining the speed of wave and its shape (for further discussion on the small parameter ϵ see [6–12]).

It is well known [9, 10] that for the conventional KPP problem without a convection term the scaling procedure $t \to t/\epsilon$, $\boldsymbol{x} \to \boldsymbol{x}/\epsilon$ yields the large-scale geometric front propagation with a velocity of the order of unity as $\epsilon \to 0$. It is tempting to suppose that there exists a scaling function $\lambda(\epsilon)$ for which the ensemble average $\langle \varphi(t/\Lambda, \boldsymbol{x}/\epsilon) \rangle$ develops the reaction front. Even though we cannot determine such ensemble average (the KPP equation (1) is nonlinear!) it is possible to find the upper bound for the ensemble averaged reaction front position and speed in the long-time, large-distance limit. Thus in this letter we are concerned with the behaviour of the set in which the ensemble average $\langle \varphi(t/\lambda, \boldsymbol{x}/\epsilon) \rangle \to 0$ in the limit $Re \to \infty$, that is $\epsilon \to 0$.

To find the ensemble averaged upper bound position

$$S_G = \{ \boldsymbol{x} \in \mathbb{R}^d \ : \ G(t, \boldsymbol{x}) = 0 \}$$

we have to determine the effective function $G(t, \boldsymbol{x})$ [6, 7]:

$$G(t, \boldsymbol{x}) = \lim_{\epsilon \to 0} \lambda(\epsilon) \ln \left\langle \varphi^* \left(\frac{t}{\lambda(\epsilon)}, \frac{\boldsymbol{x}}{\epsilon} \right) \right\rangle \qquad \boldsymbol{x} \notin \Omega. \tag{5}$$

Here φ^* is a solution of (1)–(4) when $c(\epsilon \boldsymbol{x}, \varphi)$ is replaced by its maximum value $c(\epsilon \boldsymbol{x}, 0)$.

It follows from equation (5) and the inequality $\varphi < \varphi^*$ that

$$\lim_{\epsilon \to 0} \left\langle \varphi \left(\frac{t}{\lambda(\epsilon)}, \frac{\boldsymbol{x}}{\epsilon} \right) \right\rangle = 0 \qquad \text{if} \quad G(t, \boldsymbol{x}) < 0. \tag{6}$$

To find an explicit expression for the rescaled function $\varphi^*\left(t/, \boldsymbol{x}/\epsilon\right)$ we use a functional integral technique from [9, 10].

By using the scaling transformation

$$t \to \frac{t}{\lambda(\epsilon)} \qquad \boldsymbol{x} \to \frac{\boldsymbol{x}}{\epsilon} \tag{7}$$

we can find the equation for $\varphi^*\left(t/\lambda, \boldsymbol{x}/\epsilon\right)$:

$$\frac{\partial \varphi^*}{\partial t} + \frac{\epsilon}{\lambda} \boldsymbol{v} \left(\frac{t}{\lambda}, \frac{\boldsymbol{x}}{\epsilon} \right) \nabla \varphi^* = \frac{\epsilon^2 D}{\lambda} \nabla^2 \varphi^* + \frac{1}{\lambda} c(\boldsymbol{x}, 0) \varphi^* \tag{8}$$

with the initial condition

$$\varphi^* \left(0, \frac{\boldsymbol{x}}{\epsilon} \right) = \varphi_0(\boldsymbol{x}). \tag{9}$$

Applying the Feynman–Kac formula [9, 10] we find the solution φ^* of the Cauchy problem (8), (9):

$$\varphi^*\left(\frac{t}{\lambda}, \frac{\boldsymbol{x}}{\epsilon}\right) = \mathbf{E}_x \varphi_0(\boldsymbol{x}(t)) \exp\left\{\frac{1}{\lambda}\int_0^t c(\boldsymbol{x}(s), 0)\ \mathrm{d}s\right\} \tag{10}$$

where $\mathbf{E}_x$ denotes the expectation over the trajectories $\boldsymbol{x}(t)$ that can be found from

$$\boldsymbol{x}(t) = \boldsymbol{x} - \frac{\epsilon}{\lambda}\int_0^t \boldsymbol{v}\left(\frac{t-s}{\lambda}, \frac{\boldsymbol{x}(s)}{\epsilon}\right)\mathrm{d}s + \left(\frac{2\epsilon^2 D}{\lambda}\right)^{1/2}\mathbf{W}(t). \tag{11}$$

Here $\mathbf{W}(t)$ is the standard d-dimensional Wiener process.

The solution (10) can be rewritten in an explicit form as a functional integral

$$\varphi^*\left(\frac{t}{\lambda}, \frac{\boldsymbol{x}}{\epsilon}\right) = \int \varphi_0(\boldsymbol{x}(t)) \exp\left\{\frac{1}{\lambda}\int_0^t c(\boldsymbol{x}(s), 0)\ \mathrm{d}s\right\} P[\boldsymbol{x}(s)]\ \mathcal{D}\boldsymbol{x}(s) \tag{12}$$

where the probability density functional $P[\boldsymbol{x}(s)]$ for the random process $\boldsymbol{x}(s)$ is

$$P[\boldsymbol{x}(s)] = J \exp\left\{-\frac{\lambda}{4\epsilon^2 D}\int_0^t \left(\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}s} + \frac{\epsilon}{\lambda}\boldsymbol{v}\left(\frac{t-s}{\lambda}, \frac{\boldsymbol{x}(s)}{\epsilon}\right)\right)^2 \mathrm{d}s\right\} \tag{13}$$

and the integration is performed over all trajectories starting from $\boldsymbol{x}(0) = \boldsymbol{x}$ at $s = 0$, while a suitable normalization constant is included in the definition of $\mathcal{D}\boldsymbol{x}(s)$. Since the velocity $\boldsymbol{v}$ is assumed to be solenoidal, the Jacobian $J = \exp(\alpha \int_0^t \nabla \cdot \boldsymbol{v}\, \mathrm{d}s)$ is equal to unity. Note that equation (12) with (13) is valid for any fixed realization of the random velocity field $\boldsymbol{v}$.

We next derive an ensemble average of φ^* appearing in equation (5). It is convenient to rewrite the path-integral (12) in terms of an auxiliary vector $\boldsymbol{u}(s)$ as follows [5, 13, 14]:

$$\varphi^*\left(\frac{t}{\lambda}, \frac{\boldsymbol{x}}{\epsilon}\right) = \int\!\!\int \varphi_0(\boldsymbol{x}(t)) \exp\left\{\frac{1}{\lambda}\int_0^t \left(c(\boldsymbol{x}(s), 0) - \boldsymbol{u}(s)\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}s} + \frac{\epsilon^2 D}{\lambda^2}\boldsymbol{u}^2(s)\right.\right.$$
$$\left.\left. - \frac{\epsilon}{\lambda}\boldsymbol{u}(s)\boldsymbol{v}\left(\frac{t-s}{\lambda}, \frac{\boldsymbol{x}(s)}{\epsilon}\right)\right)\mathrm{d}s\right\} \mathcal{D}\boldsymbol{x}(s)\ \mathcal{D}\left(\frac{\mathrm{i}\boldsymbol{u}(s)}{\lambda}\right). \tag{14}$$

From the well known formula for the Gaussian variable ξ with zero mean $\langle \exp a\xi \rangle = \exp\left\{\frac{1}{2}a^2\langle\xi^2\rangle\right\}$, we find that

$$\left\langle \varphi^*\left(\frac{t}{\lambda}, \frac{\boldsymbol{x}}{\epsilon}\right)\right\rangle = \int\!\!\int \varphi_0(\boldsymbol{x}(t)) \exp\left\{-\frac{1}{\lambda}\int_0^t \boldsymbol{u}\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}s}\ \mathrm{d}s\right.$$
$$\left. + \frac{1}{\lambda}H^\epsilon[\boldsymbol{x}(s), \boldsymbol{u}(s)]\right\} \mathcal{D}\boldsymbol{x}(s)\ \mathcal{D}\left(\frac{\mathrm{i}\boldsymbol{u}(s)}{\lambda}\right) \tag{15}$$

where the Hamiltonian functional H^ϵ is

$$H^\epsilon[\boldsymbol{x}(s), \boldsymbol{u}(s)] = \int_0^t \left(c(\boldsymbol{x}(s), 0) + \frac{\epsilon^2 D}{\lambda^2}\boldsymbol{u}^2\right)\mathrm{d}s$$
$$+ \frac{\epsilon^2}{2\lambda^3}\int_0^t\int_0^t \sum_{i,j}^{d} B_{ij}\left(\frac{s_1 - s_2}{\lambda}; \frac{\boldsymbol{x}(s_1)}{\epsilon}, \frac{\boldsymbol{x}(s_2)}{\epsilon}\right) u_i(s_1)u_j(s_2)\ \mathrm{d}s_1\ \mathrm{d}s_2. \tag{16}$$

These formulae, together with equation (5), allow us to find the effective function $G(t, \boldsymbol{x})$ and thereby the upper bound for the reaction front position $S_G = \{\, \boldsymbol{x} \in \mathbb{R}^d : G(t, \boldsymbol{x}) = 0 \,\}$.

The asymptotic expression for $\langle \varphi^*(t/\lambda, \boldsymbol{x}/\epsilon)\rangle$ in the limit $\epsilon \to 0$ can be written as follows:

$$\left\langle \varphi^* \left(\frac{t}{\lambda}, \frac{\boldsymbol{x}}{\epsilon} \right) \right\rangle \sim \exp\left\{ \frac{G(t, \boldsymbol{x})}{\lambda} \right\} \tag{17}$$

where

$$G(t, \boldsymbol{x}) = \sup\left\{ -\int_0^t \boldsymbol{u} \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}s}\, \mathrm{d}s + H^0 : \quad \boldsymbol{x}(0) = \boldsymbol{x},\ \boldsymbol{x}(t) \in \partial\Omega,\ \boldsymbol{x}(s) \notin \Omega \text{ for } s \in [0, t) \right\} \tag{18}$$

provided that

$$H^0 = \lim_{\epsilon \to 0} H^\epsilon$$

has a non-trivial limit.

It is clear that the functions $\boldsymbol{x}^*(s)$ and $\boldsymbol{u}^*(s)$ that maximize the functional in (18) can be found from the Hamilton variational equations

$$\frac{\mathrm{d}\boldsymbol{x}^*}{\mathrm{d}s} = \frac{\delta H^0}{\delta \boldsymbol{u}^*} \qquad \frac{\mathrm{d}\boldsymbol{u}^*}{\mathrm{d}s} = -\frac{\delta H^0}{\delta \boldsymbol{x}^*}. \tag{19}$$

Thus the entire problem of finding the upper bound position for large scale front has been reduced to maximizing the functional $-\int_0^t \boldsymbol{u}(\mathrm{d}\boldsymbol{x}/\mathrm{d}s)\,\mathrm{d}s + H^0$. However, the solutions of such variational problem cannot be found for arbitrary forms of the functions $c(\boldsymbol{x}, \boldsymbol{0})$ and $B_{ij}(t - \tau, \boldsymbol{x}, \boldsymbol{y})$. Nevetherless there are situations when this problem can be solved exactly for specific forms of c and B_{ij}.

To demonstrate the ease of application of equations (16), (18) we consider a particularly simple example: a homogeneous Gaussian random field with many spatial scales and rapid oscillations in time:

$$\langle v_i(t, \boldsymbol{x}) v_j(\tau, \boldsymbol{y})\rangle = B_{ij}(t - \tau; \boldsymbol{x}, \boldsymbol{y}) = F_{ij}^\epsilon(x - y)\delta(t - \tau). \tag{20}$$

It follows from (16) that the Hamiltonian functional H^ϵ can be written as

$$H^\epsilon = \int_0^t \left(c(\boldsymbol{x}(s), 0) + \frac{\epsilon^2 D}{\lambda^2}\boldsymbol{u}^2 + \frac{\epsilon^2}{2\lambda^2} \sum_{i,j}^{d} F_{ij}^\epsilon(0) u_i(s) u_j(s) \right) \mathrm{d}s \tag{21}$$

where the correlation tensor $F_{ij}^\epsilon(0)$ has the following asymptotic properties:

$$F_{ij}^\epsilon(0) = \begin{cases} M_{ij}\epsilon^{-\sigma} & 0 < \sigma < 2 \\ N_{ij} & \sigma < 0 \end{cases} \qquad \epsilon \to 0.$$

Here σ is a measure of the infrared divergence [7].

Consider the case in which $c(\boldsymbol{x}(s), 0) = c =$ constant, then

$$\begin{aligned} H^0 &= ct + \int_0^t h^0\, \mathrm{d}s \qquad h^0 = \frac{1}{2}\sum_{i,j=1}^{d} K_{ij} u_i(s) u_j(s) \\ K_{ij} &= \begin{cases} M_{ij} & \lambda(\epsilon) = \epsilon^{(2-\sigma)/2} \\ 2D\delta_{ij} + N_{ij} & \lambda(\epsilon) = \epsilon\,. \end{cases} \end{aligned} \tag{22}$$

To proceed further, we need an expression for the Legendre transformation of h^0, that is the Lagrangian function

$$l^0 = \sup_{\boldsymbol{u}} \left[\boldsymbol{u} \cdot \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}s} - h^0(\boldsymbol{u}) \right] = \frac{1}{2}\sum_{i,j=1}^{d} K^{ij} \frac{\mathrm{d}x_i}{\mathrm{d}s}\frac{\mathrm{d}x_j}{\mathrm{d}s} \tag{23}$$

where $K^{ij} = \left(K_{ij}\right)^{-1}$.

It follows from equations (18), (22) and (23) that

$$G(t, \boldsymbol{x}) = ct - \inf\left\{\frac{1}{2}\int_0^t \sum_{i,j=1}^{d} K^{ij}\frac{\mathrm{d}x_i}{\mathrm{d}s}\frac{\mathrm{d}x_j}{\mathrm{d}s}\,\mathrm{d}s : \right.$$

$$\left. \boldsymbol{x}(0) = \boldsymbol{x},\ \boldsymbol{x}(t) \in \partial\Omega,\ \boldsymbol{x}(s) \notin \Omega \text{ for } s \in [0, t)\right\}.$$

If we denote by ρ the Riemann metric in R^d corresponding the metric tensor $g^{ij} = K^{ij}$, [9, 10] then

$$G(t, \boldsymbol{x}) = ct - \frac{\rho^2(\boldsymbol{x}, \Omega)}{2t}$$

where the infimum is given by the minimal geodesics connecting the point $\boldsymbol{x}$ and the support Ω. Thus the upper bound for the front position is determined by

$$\rho(\boldsymbol{x}, \Omega) = t(2c)^{\frac{1}{2}}$$

while the upper bound for the velocity is given by

$$u = \left(2c\sum_{i,j=1}^{d} K^{ij} e_i e_j\right)^{\frac{1}{2}}$$

where $\boldsymbol{e}$ is the unit vector in the Euclidean metric in R^d.

In summary, this letter is a first step in the analysis of the KPP equation with a d-dimensional random velocity field with infrared divergence. It extends our previously reported works on turbulent shear flow [6, 7] (see also [8]) and contains a novel use of the functional integral technique in determining the upper bound for the ensemble averaged reaction front position and speed. The most likely future extension of this work is to investigate the influence of random velocity with Kolmogorov–Obukhov statistics [7, 15] on the propagation of the reaction front.

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