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Covariance transformations for flame-propagation modeling

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The covariance transformation used in earlier theoretical studies of turbulent-flame and isothermal-front propagation is defined and mathematically derived. This transformation provides the covariance associated with fluctuations of a turbulent scalar or vector-component variable in terms of the statistical properties of another fluctuating scalar or vector-component variable when the Fourier transforms of the two variables in transverse-wave number and frequency space are linearly dependent.

Key words: Covariance, turbulence, turbulent combustion, front propagation, flame propagation

INTRODUCTION

The potential for greatly enhanced combustion rates on one hand and safety concerns related to fire spread on the other have sustained much interest in an improved understanding of the dynamics of turbulent premixed combustion. To this end, models based on consideration of the turbulent premixed flame as an ensemble of wrinkled laminar flamelets have been useful in providing for predictions of the mean burning-rate as well as possible influences of turbulent-flame dynamics on the flow-field properties upstream and downstream from the flame (Williams, 1985). When attention is restricted to reactant flows having large overall chemical activation energies and low turbulence intensities, a Clavin-Williams quasi-planar laminar-flamelet structure may be assumed, providing for simplified solutions of the governing flow-field conservation equations and an associated evolution equation describing the flamelet dynamics (Clavin and Williams, 1982; Pelce and Clavin, 1982; Clavin and Garcia-Ybarra, 1983). Further mathematical formulation leading to solutions in terms of statistical properties of the turbulence far upstream from the flame has been useful for predicting burning speeds as well as the extent of turbulence modification near the flame, for conditions of relatively low chemical heat release (such that the laminar flamelet is intrinsically stable for all wave numbers characteristic of the excitation turbulence far upstream) (Aldredge, 1990; Aldredge and Williams, 1991). This formulation has employed the use of covariance transformations introduced in the first of these

two referenced studies and used in a more recent study of isothermal-front propagation (Aldredge, 2006) as well. These covariance transformations are defined and derived in the following section.

Formulation and derivation

Here, a general derivation of the covariance transformation theorem used in earlier theoretical analysis of turbulent-flame and isothermal-front propagation (Aldredge, 1990; Aldredge and Williams, 1991; Aldredge, 2006) is presented. The covariance transformation provides the covariance associated with fluctuations $\psi(x, y, t)$ of a turbulent scalar or vector-component variable in terms of the statistical properties of another fluctuating scalar or vector-component variable $\theta(x, y, t)$ when the Fourier transforms of ψ and θ are linearly dependent. Specifically, if a spectral transfer function $Q(x, \mathbf{k}, \omega)$ is known, such that

$$\mathfrak{F}\{\psi(x, y, t)\} = Q(x, \mathbf{k}, \omega) \mathfrak{F}\{\theta(x, y, t)\} \quad (1)$$

then

$$\left. \begin{aligned} \langle \psi^2 \rangle &= \langle \theta^2 \rangle \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathbf{k} d\omega |Q|^2 \mathfrak{F}\{\varphi\} \\ \varphi(x, \eta, \tau) &\equiv \langle \theta(x, \mathbf{y}, t) \theta(x, \mathbf{y} + \boldsymbol{\eta}, t + \tau) \rangle / \langle \theta^2 \rangle \end{aligned} \right\}; \quad (2)$$

where $\langle \rangle$ denotes the ensemble average of its argument and $\mathfrak{S}\{ \}$ represents the triple Fourier transform in transverse-wavenumber \mathbf{k} and frequency ω space, as defined by

$$\left. \begin{aligned} \Psi(x, \mathbf{k}, \omega) &= \mathfrak{S}\{\psi(x, \mathbf{y}, t)\} \equiv \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathbf{y} dt \psi(x, \mathbf{y}, t) e^{-i(\omega t + \mathbf{k} \cdot \mathbf{y})} \\ \psi(x, \mathbf{y}, t) &= \mathfrak{S}^{-1}\{\Psi(x, \mathbf{k}, \omega)\} \equiv \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathbf{k} d\omega \Psi(x, \mathbf{k}, \omega) e^{-i(\omega t + \mathbf{k} \cdot \mathbf{y})} \end{aligned} \right\} \quad (3)$$

It is assumed that the fluctuations $\theta(x, \mathbf{y}, t)$ and $\psi(x, \mathbf{y}, t)$ both exhibit stationarity and homogeneity in the transverse coordinate plane \mathbf{y} (but not necessarily along the axial coordinate direction x). More generally, considering ensemble averages involving the product of two different scalar or vector-component fluctuations ψ_A and ψ_B , we have

$$\langle \psi_A \psi_B \rangle = \theta'_A \theta'_B \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathbf{k} d\omega Q_A Q_B^* \mathfrak{S}\{\phi_{A,B}\}, \quad (4)$$

where

$$\left. \begin{aligned} \mathfrak{S}\{\psi_A(x, \mathbf{y}, t)\} &= Q_A(x, \mathbf{k}, \omega) \mathfrak{S}\{\theta_A(x, \mathbf{y}, t)\} \\ \mathfrak{S}\{\psi_B(x, \mathbf{y}, t)\} &= Q_B(x, \mathbf{k}, \omega) \mathfrak{S}\{\theta_B(x, \mathbf{y}, t)\} \\ \phi_{A,B}(x, \eta, \tau) &\equiv \langle \theta_A(x, \mathbf{y}, t) \theta_B(x, \mathbf{y} + \boldsymbol{\eta}, t + \tau) \rangle / \theta'_A \theta'_B \\ \theta'_A &\equiv \langle \theta_A^2 \rangle^{1/2}, \quad \theta'_B \equiv \langle \theta_B^2 \rangle^{1/2} \end{aligned} \right\}; \quad (5)$$

and the superscript $*$ signifies that the complex conjugate is taken. We will now prove Eq. (4) defining the general form of the covariance transformation theorem, with the first relation of Eq. (2) representing one of two special cases.

Application of the inverse Fourier-transform operator $\mathfrak{S}^{-1}\{ \}$, as defined by the second relation in Equation (3), to Equation (1) results in the following well-known convolution theorem.

$$\psi(x, \mathbf{y}, t) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\boldsymbol{\eta} d\tau q(x, \boldsymbol{\eta}, \tau) \theta(x, \mathbf{y} - \boldsymbol{\eta}, t - \tau), \quad (6)$$

where $q(x, \mathbf{y}, t) \equiv \mathfrak{S}^{-1}\{Q\}$. Hence, one has

$$\begin{aligned} \langle \psi_A \psi_B \rangle &= \frac{1}{(2\pi)^6} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\boldsymbol{\eta}_A d\tau_A d\boldsymbol{\eta}_B d\tau_B \\ &\quad \times q_A(x, \boldsymbol{\eta}_A, \tau_A) q_B(x, \boldsymbol{\eta}_B, \tau_B) \\ &\quad \times \langle \theta_A(x, \mathbf{y} - \boldsymbol{\eta}_A, t - \tau_A) \theta_B(x, \mathbf{y} - \boldsymbol{\eta}_B, t - \tau_B) \rangle \end{aligned} \quad (7)$$

which, due to the assumed conditions of turbulence stationarity and transverse homogeneity, becomes;

$$\begin{aligned} \langle \psi_A \psi_B \rangle &= \frac{\theta'_A \theta'_B}{(2\pi)^6} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\boldsymbol{\eta}_A d\tau_A d\boldsymbol{\eta}_B d\tau_B \\ &\quad \times q_A(x, \boldsymbol{\eta}_A, \tau_A) q_B(x, \boldsymbol{\eta}_B, \tau_B) \phi_{A,B}(x, |\boldsymbol{\eta}_B - \boldsymbol{\eta}_A|, |\tau_B - \tau_A|) \end{aligned} \quad (8)$$

Upon introduction of the new variables $\boldsymbol{\eta} \equiv \boldsymbol{\eta}_B - \boldsymbol{\eta}_A$ and $\tau \equiv \tau_B - \tau_A$, we then have

$$\begin{aligned} \langle \psi_A \psi_B \rangle &= \frac{\theta'_A \theta'_B}{(2\pi)^6} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\boldsymbol{\eta} d\tau \phi_{A,B}(x, \boldsymbol{\eta}, \tau) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\boldsymbol{\eta}_A d\tau_A q_A(x, \boldsymbol{\eta}_A, \tau_A) \\ &\quad \times q_B(x, \boldsymbol{\eta} + \boldsymbol{\eta}_A, \tau + \tau_A) \end{aligned} \quad (9)$$

Since it can be easily shown that

$$\begin{aligned} &\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\boldsymbol{\eta}_A d\tau_A q_A(x, \boldsymbol{\eta}_A, \tau_A) q_B(x, \boldsymbol{\eta} + \boldsymbol{\eta}_A, \tau + \tau_A) \\ &= (2\pi)^3 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathbf{k} d\omega Q_A(x, \mathbf{k}, \omega) Q_B^*(x, \mathbf{k}, \omega) e^{-i(\omega\tau + \mathbf{k} \cdot \boldsymbol{\eta})} \end{aligned} \quad (10)$$

by substitution of integral expressions for $q_A \equiv \mathfrak{S}^{-1}\{Q_A\}$ and $q_B \equiv \mathfrak{S}^{-1}\{Q_B\}$, according to the second relation of Equation (3), and use of the properties of the well known Dirac delta function, δ_D , defined here by

$$\delta_D(\mathbf{k}, \omega) \equiv \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\boldsymbol{\eta} d\tau e^{i(\omega\tau + \mathbf{k} \cdot \boldsymbol{\eta})}. \quad (11)$$

Therefore, Eq. (9) becomes

$$\begin{aligned} \langle \psi_A \psi_B \rangle &= \frac{\theta'_A \theta'_B}{(2\pi)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathbf{k} d\omega Q_A(x, \mathbf{k}, \omega) \\ &\quad \times Q_B^*(x, \mathbf{k}, \omega) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\boldsymbol{\eta} d\tau e^{-i(\omega\tau + \mathbf{k} \cdot \boldsymbol{\eta})} \phi_{A,B}(x, \boldsymbol{\eta}, \tau) \end{aligned}, \quad (12)$$

which is equivalent to Eq. (4) since

$$\mathfrak{S}\{\phi_{AB}\} = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\boldsymbol{\eta} d\tau e^{-i(\omega\tau + \mathbf{k} \cdot \boldsymbol{\eta})} \phi_{A,B}(x, \boldsymbol{\eta}, \tau). \quad (13)$$

The special case of Eq. (2) relating the autocorrelations $\langle \psi^2 \rangle$ and $\langle \theta^2 \rangle$ follows directly from the more general form in Eq. (4), after elimination of the subscripts and use of the identity $|Q|^2 = QQ^*$.

Lastly, we derive the covariance transformation giving $\langle \psi^2 \rangle$ when the spectral transfer function is a vector $\mathbf{Q} \equiv (Q_m, Q_n)$ in transverse wavenumber space such that;

$$\mathfrak{S}\{\psi(x, \mathbf{y}, t)\} = \mathbf{Q}(x, \mathbf{k}, \omega) \cdot \mathfrak{S}\{\boldsymbol{\theta}(x, \mathbf{y}, t)\}. \quad (14)$$

In this case one has [c.f., Eq. (6)]

$$\psi(x, y, t) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\boldsymbol{\eta} d\boldsymbol{\tau} \mathbf{q}(x, \boldsymbol{\eta}, \boldsymbol{\tau}) \cdot \boldsymbol{\theta}(x, \mathbf{y} - \boldsymbol{\eta}, t - \boldsymbol{\tau}), \quad (15)$$

and consequently

$$\langle \psi^2 \rangle = \frac{1}{(2\pi)^6} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\boldsymbol{\eta}_A d\boldsymbol{\tau}_A d\boldsymbol{\eta}_B d\boldsymbol{\tau}_B \times \left\{ \begin{aligned} &\langle \theta_m^2 \rangle q_m(x, \boldsymbol{\eta}_A, \boldsymbol{\tau}_A) q_m(x, \boldsymbol{\eta}_B, \boldsymbol{\tau}_B) \varphi_{m,m}(x, |\boldsymbol{\eta}_B - \boldsymbol{\eta}_A|, |\boldsymbol{\tau}_B - \boldsymbol{\tau}_A|) \\ &+ \langle \theta_n^2 \rangle q_n(x, \boldsymbol{\eta}_A, \boldsymbol{\tau}_A) q_n(x, \boldsymbol{\eta}_B, \boldsymbol{\tau}_B) \varphi_{n,n}(x, |\boldsymbol{\eta}_B - \boldsymbol{\eta}_A|, |\boldsymbol{\tau}_B - \boldsymbol{\tau}_A|) \\ &+ \theta'_m \theta'_n q_m(x, \boldsymbol{\eta}_A, \boldsymbol{\tau}_A) q_n(x, \boldsymbol{\eta}_B, \boldsymbol{\tau}_B) \varphi_{m,n}(x, |\boldsymbol{\eta}_B - \boldsymbol{\eta}_A|, |\boldsymbol{\tau}_B - \boldsymbol{\tau}_A|) \\ &+ \theta'_m \theta'_n q_n(x, \boldsymbol{\eta}_A, \boldsymbol{\tau}_A) q_m(x, \boldsymbol{\eta}_B, \boldsymbol{\tau}_B) \varphi_{n,m}(x, |\boldsymbol{\eta}_B - \boldsymbol{\eta}_A|, |\boldsymbol{\tau}_B - \boldsymbol{\tau}_A|) \end{aligned} \right\} \quad (16)$$

After introducing the new variables $\boldsymbol{\eta} \equiv \boldsymbol{\eta}_b - \boldsymbol{\eta}_a$ and $\boldsymbol{\tau} \equiv \boldsymbol{\tau}_b - \boldsymbol{\tau}_a$, we then obtain

$$\langle \psi^2 \rangle = \frac{1}{(2\pi)^6} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\boldsymbol{\eta} d\boldsymbol{\tau} d\boldsymbol{\eta}_A d\boldsymbol{\tau}_A \times \left\{ \begin{aligned} &\langle \theta_m^2 \rangle q_m(x, \boldsymbol{\eta}_A, \boldsymbol{\tau}_A) q_m(x, \boldsymbol{\eta} + \boldsymbol{\eta}_A, \boldsymbol{\tau} + \boldsymbol{\tau}_A) \varphi_{m,m}(x, \boldsymbol{\eta}, \boldsymbol{\tau}) \\ &+ \langle \theta_n^2 \rangle q_n(x, \boldsymbol{\eta}_A, \boldsymbol{\tau}_A) q_n(x, \boldsymbol{\eta} + \boldsymbol{\eta}_A, \boldsymbol{\tau} + \boldsymbol{\tau}_A) \varphi_{n,n}(x, \boldsymbol{\eta}, \boldsymbol{\tau}) \\ &+ \theta'_m \theta'_n q_m(x, \boldsymbol{\eta}_A, \boldsymbol{\tau}_A) q_n(x, \boldsymbol{\eta} + \boldsymbol{\eta}_A, \boldsymbol{\tau} + \boldsymbol{\tau}_A) \varphi_{m,n}(x, \boldsymbol{\eta}, \boldsymbol{\tau}) \\ &+ \theta'_m \theta'_n q_n(x, \boldsymbol{\eta}_A, \boldsymbol{\tau}_A) q_m(x, \boldsymbol{\eta} + \boldsymbol{\eta}_A, \boldsymbol{\tau} + \boldsymbol{\tau}_A) \varphi_{n,m}(x, \boldsymbol{\eta}, \boldsymbol{\tau}) \end{aligned} \right\} \quad (17)$$

and then [c.f., Eq. (10)]

$$\langle \psi^2 \rangle = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathbf{k} d\boldsymbol{\omega} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\boldsymbol{\eta} d\boldsymbol{\tau} e^{-i(\boldsymbol{\omega}\boldsymbol{\tau} + \mathbf{k}\boldsymbol{\eta})} \times \left\{ \begin{aligned} &\langle \theta_m^2 \rangle |Q_m(x, \mathbf{k}, \boldsymbol{\omega})|^2 \varphi_{m,m}(x, \boldsymbol{\eta}, \boldsymbol{\tau}) \\ &+ \langle \theta_n^2 \rangle |Q_n(x, \mathbf{k}, \boldsymbol{\omega})|^2 \varphi_{n,n}(x, \boldsymbol{\eta}, \boldsymbol{\tau}) \\ &+ \theta'_m \theta'_n Q_m(x, \mathbf{k}, \boldsymbol{\omega}) Q_n^*(x, \mathbf{k}, \boldsymbol{\omega}) \varphi_{m,n}(x, \boldsymbol{\eta}, \boldsymbol{\tau}) \\ &+ \theta'_m \theta'_n Q_n^*(x, \mathbf{k}, \boldsymbol{\omega}) Q_m(x, \mathbf{k}, \boldsymbol{\omega}) \varphi_{n,m}(x, \boldsymbol{\eta}, \boldsymbol{\tau}) \end{aligned} \right\}. \quad (18)$$

Finally, this result is equivalent to

$$\langle \psi^2 \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathbf{k} d\boldsymbol{\omega} \times \left[\langle \theta_m^2 \rangle |Q_m|^2 \mathfrak{S}\{\varphi_{m,m}\} + \langle \theta_n^2 \rangle |Q_n|^2 \mathfrak{S}\{\varphi_{n,n}\} + \theta'_m \theta'_n (Q_m Q_n^* \mathfrak{S}\{\varphi_{m,n}\} + Q_m^* Q_n \mathfrak{S}\{\varphi_{n,m}\}) \right] \quad (19)$$

for the case where

$$\mathfrak{S}\{\psi(x, \mathbf{y}, t)\} = Q_m(x, \mathbf{k}, \boldsymbol{\omega}) \mathfrak{S}\{\theta_m(x, \mathbf{y}, t)\} + Q_n(x, \mathbf{k}, \boldsymbol{\omega}) \mathfrak{S}\{\theta_n(x, \mathbf{y}, t)\} \quad (20)$$

is stipulated [c.f., Eq. (14)]. Extending the theorem to the case where the Fourier transform of $\psi(x, \mathbf{y}, t)$ depends on

an arbitrary number J of spectral-field components, is stipulated [c.f., Eq. (14)]. Extending the theorem to the case where the Fourier transform of $\psi(x, \mathbf{y}, t)$ depends on an arbitrary number J of spectral-field components, such that;

$$\mathfrak{S}\{\psi(x, \mathbf{y}, t)\} = \sum_{j=1}^J Q_j(x, \mathbf{k}, \boldsymbol{\omega}) \mathfrak{S}\{\theta_j(x, \mathbf{y}, t)\}, \quad (21)$$

it can be easily shown that

$$\langle \psi^2 \rangle = \sum_{j=1}^J \sum_{i=1}^J \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathbf{k} d\boldsymbol{\omega} \theta'_i \theta'_j Q_i Q_j^* \mathfrak{S}\{\varphi_{i,j}\}; \quad (22)$$

which reduces to Eq. (19) when $J = 2$.

Summary

In summary, the general form of the covariance transformation theorem, providing $\langle \psi_A \psi_B \rangle$ in terms of the statistical properties of θ_A and θ_B when the Fourier transform of ψ_A (ψ_B) is proportional to that of θ_A (θ_B), is given by Equations (4) and (5). The form of the transformation providing the autocovariance $\langle \psi^2 \rangle$ (for the special case where $\psi_A = \psi_B$ and $\theta_A = \theta_B$) is given explicitly in Equations (1) and (2). Another special case, providing the autocovariance $\langle \psi^2 \rangle$ when $\mathfrak{S}\{\psi\}$ is the weighted sum of two linearly independent spectral-field components, is given by Equations (19) and (20); while an extension of this result for the case where $\mathfrak{S}\{\psi\}$ depends on an arbitrary number J of linearly independent spectral-field components is provided in Equations (21) and (22).

The covariance transformations defined and derived in the present work are useful in mathematical formulations of turbulent flame propagation which relate properties of the turbulent flame (e.g., its speed and structure) to the properties of the reactant mixture through which the flame propagates (e.g., turbulence intensity, length and time scales and energy distribution). Such formulations can allow improved understanding of turbulent flame propagation and ultimately the potential for greatly enhanced combustion rates and improved fire safety.

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