

STRUCTURE OF THE REACTANT AND PRODUCT OF A TURBULENT FIRST ORDER REACTION AT LARGE WAVE-NUMBERS

by PREM KUMAR and YASH PAUL, *Department of Mathematics,
Indian Institute of Technology, New Delhi 29*

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The simple continuous spectral cascading process for the transfer of turbulent kinetic energy, heat and mass at large wave-numbers as presented by Pao (1965) has been applied to find the spectrum functions of the reactant and the product of reaction field concentration for different spectral ranges. Under the restrictions (i) that the flow field and the scalar field are stationary, (ii) the Kolmogorov's hypothesis that the small-scale structure turbulence is statistically steady and isotropic, (iii) that the small-scale structure of scalar field is statistically steady and isotropic, the results are obtained in a closed form.

INTRODUCTION

Obukhov (1949) and Corrsin (1951) extended the Kolmogorov's second hypothesis to investigate the small-scale structure of the fluctuating scalar field. Again following the technique of Onsager (1949) and the mixing theories of Batchelor (1959) and Batchelor *et al.* (1959), Corrsin (1961) estimated the form of the first order reactant concentration power spectrum in the stationary and locally isotropic case for various Schmidt numbers and spectral ranges. Some of the properties of the product of reaction field concentration have been discussed by Corrsin (1962). Recently Pao (1965) has proposed a simple continuous spectral cascading process for the transfer of turbulent kinetic energy, heat and mass at large wave-numbers. Based on these concepts, he obtains energy, temperature and concentration spectrum functions for the whole universal range. In the present paper, we apply Pao's concepts to obtain spectrum functions of the reactant and the product of reaction field concentration for different spectral ranges. The results, so obtained, have been compared with the results obtained by other workers in the field.

BASIC EQUATIONS

The equations governing the isothermal constant density flow with dilute diffusive scalar quantity $\Theta(\vec{x}, t)$ are

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = - \frac{1}{\rho} \frac{\partial P}{\partial x_i} + \nu \frac{\partial^2 U_i}{\partial x_j^2} \quad (\text{conservation of momentum}) \quad \dots \quad (1)$$

$$\frac{\partial U_i}{\partial x_i} = 0 \quad (\text{conservation of mass}) \quad \dots \dots \dots (2)$$

$$\frac{\partial \Theta}{\partial t} + U_i \frac{\partial \Theta}{\partial x_i} = D \frac{\partial^2 \Theta}{\partial x_i^2} - C\Theta \quad (\text{conservation of reactant}) \quad \dots \dots (3)$$

$$\frac{\partial \Gamma}{\partial t} + U_i \frac{\partial \Gamma}{\partial x_i} = D_1 \frac{\partial^2 \Gamma}{\partial x_i^2} + C\Theta \quad (\text{conservation of the product of reaction}) \quad (4)$$

where U_i is the velocity vector, P is the pressure, ρ is the constant density, ν is the constant kinematic viscosity, $\Theta(\vec{x}, t)$, $\Gamma(\vec{x}, t)$ are the concentrations of the reactant and the product of reaction respectively, D and D_1 are the diffusivities of the reactant and the product of reaction respectively.

Assuming (i) that the flow field and the scalar fields are stationary, (ii) Kolmogorov's hypothesis that the small-scale structure of turbulence is statistically steady and isotropic, (iii) that the small-scale structure of scalar field is statistically steady and isotropic (the extension of Kolmogorov's hypothesis to the scalar field), (iv) that the observer moves with the mean velocity \bar{U}_j ; and following Pao (1965), we find the equations in terms of the fluctuating quantities as

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j^2} \quad \dots \dots \dots (5)$$

$$\frac{\partial u_i}{\partial x_i} = 0 \quad \text{for } |\vec{x}' - \vec{x}| < l_v \quad \dots \dots \dots (6)$$

$$\frac{\partial \theta}{\partial t} + u_i \frac{\partial \theta}{\partial x_i} = D \frac{\partial^2 \theta}{\partial x_i^2} - C\theta \quad \dots \dots \dots (7)$$

$$\frac{\partial \gamma}{\partial t} + u_i \frac{\partial \gamma}{\partial x_i} = D_1 \frac{\partial^2 \gamma}{\partial x_i^2} + C\theta \quad \text{for } |\vec{x}' - \vec{x}| < l_s \quad \dots \dots \dots (8)$$

where

$$U_i = \bar{U}_i + u_i, \quad \Gamma = \bar{\Gamma} + \gamma, \quad \Theta = \bar{\Theta} + \theta \\ P = \bar{P} + p; \quad \bar{U}_i, \bar{\Gamma}, \bar{\Theta}, \bar{P}$$

being the ensemble means and u_i , θ , γ , p being the fluctuations about their respective means; l_v , l_s (smaller of l_θ , l_γ) being the characteristic lengths for the small region considered. It may be noted that, though eqns. (5) to (8) seem to be the same as for homogeneous turbulence, they are valid for the small region $|\vec{x}' - \vec{x}| < l_v$, $|\vec{x}' - \vec{x}| < l_s$.

COVARIANCE EQUATIONS

Since we are interested in knowing the behaviour of the reactant and the product of reaction, therefore, we consider eqns. (7) and (8). Here we consider the simplest case of a chemical system for which the diffusivities are equal, i.e.

$D = D_1$. It means that both the concentrations (viz. the reactant concentration and the concentration of the product of reaction) diffuse together, i.e. it is not possible for one to diffuse and for the other not to diffuse. If they diffuse, they will always diffuse together. Then eqns. (7) and (8) can be written as

$$\frac{\partial \theta}{\partial t} + u_i \frac{\partial \theta}{\partial x_i} = D \frac{\partial^2 \theta}{\partial x_i^2} - C\theta \quad \dots \quad (9)$$

$$\frac{\partial \gamma}{\partial t} + u_i \frac{\partial \gamma}{\partial x_i} = D \frac{\partial^2 \gamma}{\partial x_i^2} + C\theta. \quad \dots \quad (10)$$

Addition of (9) and (10) gives

$$\frac{\partial \sigma}{\partial t} + u_i \frac{\partial \sigma}{\partial x_i} = D \frac{\partial^2 \sigma}{\partial x_i^2} \quad \dots \quad (11)$$

where

$$\sigma \equiv \theta + \gamma.$$

Following Hinze (1959), the covariance equations for various combinations can be obtained in the usual way as

$$\overline{(u'_i - u_i) \frac{\partial}{\partial r_i} (\sigma \sigma')} = 2D \frac{\partial^2 \overline{\sigma \sigma'}}{\partial r_i^2} \quad \dots \quad (12)$$

$$\overline{(u'_i - u_i) \frac{\partial}{\partial r_i} (\theta \theta')} = 2D \frac{\partial^2 \overline{\theta \theta'}}{\partial r_i^2} - 2C \overline{\theta \theta'} \quad \dots \quad (13)$$

$$\overline{(u'_i - u_i) \frac{\partial}{\partial r_i} (\gamma \gamma')} = 2D \frac{\partial^2 \overline{\gamma \gamma'}}{\partial r_i^2} + 2C \overline{\theta \gamma'} \quad \dots \quad (14)$$

$$\overline{(u'_i - u_i) \frac{\partial}{\partial r_i} (\theta \gamma')} = 2D \frac{\partial^2 \overline{\theta \gamma'}}{\partial r_i^2} - C \overline{\theta \gamma'} + C \overline{\theta \theta'} \quad \dots \quad (15)$$

where quantities with a prime are the quantities at the point $\vec{x}' = \vec{x} + \vec{r}$. As the fields are stationary and isotropic, therefore, we have taken

$$\frac{\partial}{\partial t} \overline{\theta \theta'} = \frac{\partial}{\partial t} \overline{\gamma \gamma'} = \frac{\partial}{\partial t} \overline{\sigma \sigma'} = \frac{\partial}{\partial t} \overline{\theta \gamma'} = 0$$

and

$$\overline{\theta \gamma'} = \overline{\theta' \gamma}.$$

From the definition of σ , we have

$$\overline{\sigma \sigma'} = \overline{\theta \theta'} + \overline{\gamma \gamma'} + 2\overline{\theta \gamma'}. \quad \dots \quad (16)$$

Equations (12) to (16) in wave-number space are rewritten as

$$Z_1(k) = 2Dk^2 F_1(k) \quad \dots \quad (17)$$

$$Z_2(k) = 2Dk^2 F_2(k) + 2CF_2(k) \quad \dots \quad (18)$$

$$Z_3(k) = 2Dk^2 F_3(k) - 2CF_4(k) \quad \dots \quad (19)$$

$$Z_4(k) = 2Dk^2 F_4(k) + CF_4(k) - CF_2(k) \quad \dots \quad (20)$$

$$F_1(k) = F_2(k) + F_3(k) + 2F_4(k) \quad \dots \quad (21)$$

where

$$Z_1(k) = \frac{2}{\pi} \int_0^\infty \overline{(u_i - u'_i) \frac{\partial}{\partial r_i} (\sigma \sigma')} kr \sin kr \, dr$$

$$Z_2(k) = \frac{2}{\pi} \int_0^\infty \overline{(u_i - u'_i) \frac{\partial}{\partial r_i} (\theta \theta')} kr \sin kr \, dr$$

$$Z_3(k) = \frac{2}{\pi} \int_0^\infty \overline{(u_i - u'_i) \frac{\partial}{\partial r_i} (\gamma \gamma')} kr \sin kr \, dr$$

$$Z_4(k) = \frac{2}{\pi} \int_0^\infty \overline{(u_i - u'_i) \frac{\partial}{\partial r_i} (\theta \gamma')} kr \sin kr \, dr$$

$$F_1(k) = \frac{2}{\pi} \int_0^\infty \overline{\sigma \sigma'} kr \sin kr \, dr$$

$$F_2(k) = \frac{2}{\pi} \int_0^\infty \overline{\theta \theta'} kr \sin kr \, dr$$

$$F_3(k) = \frac{2}{\pi} \int_0^\infty \overline{\gamma \gamma'} kr \sin kr \, dr$$

$$F_4(k) = \frac{2}{\pi} \int_0^\infty \overline{\theta \gamma'} kr \sin kr \, dr.$$

Here $Z_r(k)$ ($r = 1, 2, 3, 4$) give the contributions due to turbulent convective transfer of $\overline{\sigma^2}$, $\overline{\theta^2}$, $\overline{\gamma^2}$, $\overline{\theta \gamma}$ contents from all other wave-numbers. The rates at which the spectral contributions of these quantities in wave-number space from wave-numbers less than k to wave-numbers greater than k are

$$Y_r(k) = \int_k^\infty Z_r(k) \, dk \quad (r = 1, 2, 3, 4)$$

which give

$$-\frac{dY_r(k)}{dk} = Z_r(k) \quad (r = 1, 2, 3, 4). \quad \dots \quad (22)$$

As in the case of pure mixing discussed by Pao (1965), we consider the migration of the scalar elements in the universal range, $k \gg ks$ where $ks = L_s^{-1}$, L_s being the smaller of the integral length scales L_θ and L_γ of the scalar fields θ and γ .

Assuming $s(k) = \frac{dk}{d\tau}$ to be the rate of transport of the spectral element across the wave-number k , the rates at which the spectral contributions of the quantities $\overline{\sigma^2}$, $\overline{\theta^2}$, $\overline{\gamma^2}$, $\overline{\theta \gamma}$ from wave-numbers less than k to wave-numbers greater than k can be obtained from

$$Y_r(k) = s(k)F_r(k) \quad (r = 1, 2, 3, 4). \quad \dots \quad (23)$$

UNIVERSAL EQUILIBRIUM RANGE

Cascading of $\overline{\sigma^2}$, $\overline{\theta^2}$, $\overline{\gamma^2}$, $\overline{\theta\gamma}$ contents is due to the turbulent convection which is dependent on the energy flux ϵ supplied by the large eddies to the small eddies. We assume that $s(k)$ is dependent on ϵ and k , and take

$$s(k) = n^{-1}\epsilon^{1/3}k^{5/3} \quad \dots \quad \dots \quad \dots \quad (24)$$

as taken by Pao (1965), where n is some dimensionless constant. Thus the relations (23) for the universal equilibrium range give

$$Y_r(k) = F_r(k)s(k) = n^{-1}\epsilon^{1/3}k^{5/3}F_r(k) \quad (r = 1, 2, 3, 4). \quad \dots \quad (25)$$

Combining eqns. (17) to (20) with relations (23) and (25), we get

$$-\frac{d}{dk}(n^{-1}\epsilon^{1/3}k^{5/3}F_1) = 2Dk^2F_1 \quad \dots \quad \dots \quad \dots \quad (26)$$

$$-\frac{d}{dk}(n^{-1}\epsilon^{1/3}k^{5/3}F_2) = 2(Dk^2 + C)F_2 \quad \dots \quad \dots \quad \dots \quad (27)$$

$$-\frac{d}{dk}(n^{-1}\epsilon^{1/3}k^{5/3}F_3) = 2Dk^2F_3 - 2CF_4 \quad \dots \quad \dots \quad \dots \quad (28)$$

$$-\frac{d}{dk}(n^{-1}\epsilon^{1/3}k^{5/3}F_4) = 2Dk^2F_4 + CF_4 - CF_2. \quad \dots \quad \dots \quad (29)$$

These are ordinary differential equations. After simplifying and using (21), the solutions of eqns. (26) to (29) are obtained as

$$F_1(k) = Q_1k^{-5/3} \exp(-3/2pk^{4/3}) \quad \dots \quad \dots \quad \dots \quad \dots \quad (30)$$

$$F_2(k) = Q_2k^{-5/3} \exp(-3/2pk^{4/3} + 3qk^{-2/3}) \quad \dots \quad \dots \quad \dots \quad \dots \quad (31)$$

$$F_3(k) = \{Q_1 + Q_2 \exp(3qk^{-2/3}) - 2Q_3 \exp(3/2qk^{-2/3})\}k^{-5/3} \exp(-3/2pk^{4/3}) \quad \dots \quad (32)$$

$$F_4(k) = \{Q_3 - Q_2 \exp(3/2qk^{-2/3})\}k^{-5/3} \exp(-3/2pk^{4/3} + 3/2qk^{-2/3}) \quad \dots \quad (33)$$

where

$$p = nD\epsilon^{-1/3}, \quad q = nC\epsilon^{-1/3}$$

$$Q_1 = F_1(k_*)k_*^{5/3} \exp(3/2pk_*^{4/3})$$

$$Q_2 = F_2(k_*)k_*^{5/3} \exp(3/2pk_*^{4/3} - 3qk_*^{-2/3})$$

$$Q_3 = \{F_2(k_*) + F_4(k_*)\}k_*^{5/3} \exp(3/2pk_*^{4/3} - 3/2qk_*^{-2/3})$$

k_* being any wave-number in the universal range.

The results (30), (31) and (32) give $\overline{\sigma^2}$, $\overline{\theta^2}$ and $\overline{\gamma^2}$ spectrum respectively.

The result (31) is the same as the result (12) derived by Corrsin (1964) for the case of inertial diffusive range with isothermal first order reaction. From this relation we see that $\overline{\theta^2}$ spectrum is related to the non-reactive mixing result by

$$F_2(k) = (Q_2)_{c=0}k^{-5/3} \exp(-3/2pk^{4/3}) \exp(3qk^{-2/3}) \sim F_{2M} \times \exp(3qk^{-2/3}) \quad \dots \quad (34)$$

where F_{2M} denotes the $\overline{\theta^2}$ spectrum for the case of pure mixing only.

It is interesting to note that the spectrum of the product of reaction concentration as given by (32) and the $\bar{\theta}^2$ spectrum as given by (31) become same when there is no chemical reaction. This should be so because for pure mixing case the basic eqns. (9) and (10) become identical.

INERTIAL CONVECTIVE RANGE

In this range, the effects due to viscosity and diffusivity are unimportant. Therefore, the diffusive and the viscous terms can be neglected. In this case also, $s(k)$ depends on ϵ and k . Therefore, for $s(k)$ we can again take the relation (24). The relation (25) is valid for this range also. Under these conditions, eqns. (26) to (29) take the simpler forms

$$-\frac{d}{dk}(n^{-1}\epsilon^{1/3}k^{5/3}F_1) = 0 \quad \dots \quad (35)$$

$$-\frac{d}{dk}(n^{-1}\epsilon^{1/3}k^{5/3}F_2) = 2CF_2 \quad \dots \quad (36)$$

$$-\frac{d}{dk}(n^{-1}\epsilon^{1/3}k^{5/3}F_3) = -2CF_4 \quad \dots \quad (37)$$

$$-\frac{d}{dk}(n^{-1}\epsilon^{1/3}k^{5/3}F_4) = CF_4 - CF_2 \quad \dots \quad (38)$$

The solutions of these equations are found to be

$$F_1(k) = A_1k^{-5/3} \quad \dots \quad (39)$$

$$F_2(k) = A_2k^{-5/3} \exp(3qk^{-2/3}) \quad \dots \quad (40)$$

$$F_3(k) = \{A_1 + A_2 \exp(3qk^{-2/3}) - 2A_3 \exp(3/2qk^{-2/3})\}k^{-5/3} \quad \dots \quad (41)$$

$$F_4(k) = \{A_3 - A_2 \exp(3/2qk^{-2/3})\}k^{-5/3} \exp(3/2qk^{-2/3}) \quad \dots \quad (42)$$

where

$$q = nC\epsilon^{-1/3}$$

$$A_1 = F_1(k_\dagger)k_\dagger^{5/3}$$

$$A_2 = F_2(k_\dagger)k_\dagger^{5/3} \exp(-3qk_\dagger^{-2/3})$$

$$A_3 = \{F_2(k_\dagger) + F_4(k_\dagger)\}k_\dagger^{5/3} \exp(-3/2qk_\dagger^{-2/3})$$

k_\dagger being any wave-number in the inertial convective range.

The result (40) is the same as the result (23) of Corrsin (1961). For pure mixing case $F_2(k)$ and $F_3(k)$, the spectra of the $\bar{\theta}^2$ and $\bar{\gamma}^2$ contents become identical as $\sim k^{-5/3}$. It is again due to the fact that the fundamental equations governing these spectra become identical.

VISCOUS-CONVECTIVE AND VISCOUS-DIFFUSIVE RANGE

In this range for large Schmidt numbers Batchelor's idea (1959), that the transfer of spectral content is mainly controlled by the straining motion

associated with small eddies, can very well be applied. Then $s(k)$ depends on the local least turbulent straining rate q (say). On dimensional basis:

$$s(k) = lqk \quad \dots \quad \dots \quad \dots \quad \dots \quad (43)$$

where l is some dimensionless constant. Thus, in this case, the eqns. (26) to (29) take the forms

$$-\frac{d}{dk}(lqkF_1) = 2Dk^2F_1 \quad \dots \quad \dots \quad \dots \quad \dots \quad (44)$$

$$-\frac{d}{dk}(lqkF_2) = 2(Dk^2 + C)F_2 \quad \dots \quad \dots \quad \dots \quad \dots \quad (45)$$

$$-\frac{d}{dk}(lqkF_3) = 2Dk^2F_3 - 2CF_4 \quad \dots \quad \dots \quad \dots \quad \dots \quad (46)$$

$$-\frac{d}{dk}(lqkF_4) = 2Dk^2F_4 + CF_4 - CF_2 \quad \dots \quad \dots \quad \dots \quad \dots \quad (47)$$

The solutions of these equations are

$$F_1(k) = B_1k^{-1} \exp(-ak^2) \quad \dots \quad \dots \quad \dots \quad \dots \quad (48)$$

$$F_2(k) = B_2k^{-(1+2b)} \exp(-ak^2) \quad \dots \quad \dots \quad \dots \quad \dots \quad (49)$$

$$F_3(k) = \{B_1 + B_2k^{-2b} - 2B_3k^{-b}\}k^{-1} \exp(-ak^2) \quad \dots \quad \dots \quad (50)$$

$$F_4(k) = \{B_3 - B_2k^{-b}\}k^{-(1+b)} \exp(-ak^2) \quad \dots \quad \dots \quad \dots \quad (51)$$

where

$$a = D/lq, \quad b = C/lq$$

$$B_1 = F_1(k_0)k_0 \exp(ak_0^2)$$

$$B_2 = F_2(k_0)k_0^{(1+2b)} \exp(ak_0^2)$$

$$B_3 = \{F_2(k_0) + F_4(k_0)\}k_0^{(1+b)} \exp(ak_0^2)$$

k_0 being the wave-number marking the beginning of viscous-convective range. For $l = -1$, the result (49) is identical with the result (46) of Corrsin (1961).

In the inertial diffusive range for small Schmidt numbers, as the energy spectrum is still in the inertial convective range, therefore $s(k)$ is the same as (24). All the results obtained for universal equilibrium range are valid for this range also.

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