

Study of Statistical Quantities of Turbulence with Reacting and Mixing Chemical Elements of the Type $A+B \rightarrow \text{Product}$

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Abstract: The governing equations for the description of turbulence with reacting and mixing n-chemical elements described by R. S. Brodkey and E. E. O'Brien are considered. The turbulent reaction mixture with reacting and mixing chemical elements consists of irreversible, isothermic, second order reaction and the type of reactions is $A+B \rightarrow \text{Product}$. These governing equations of motion are written in Fourier space. On considering the Lewis-Kraichnan space-time version of Hopf functional formalism for the investigation of turbulence under study we define the characteristic functional (or moment generating functional) for the joint probability distribution of the velocity vector of the flow field and the reactants' concentration scalar field. The equations for kinetic energy spectrum density function and concentration field obtained on employing multiple-scale-cumulant-expansion (MSCE) method forms the basis for applications of Factorized-Cumulant-Expansion-Approximation (FCEA) method. N. E. Joshi and M. C. Meshram on considering multiple-scale-cumulant-expansion (MSCE) method obtained a closed set of equations for cumulants and derived the equations for kinetic energy spectrum density function and concentration field. Therefore, for employing the FCEA method for present investigation the equations for kinetic energy spectrum density function and concentration field as obtained by them are first selected. These equations are further written on employing FCEA method. Thereafter, these equations are first written in dimensionless form and then integrated numerically. The values of energy of velocity field and concentration field are used to evaluate the statistical quantities describing the turbulence with reacting and mixing chemical elements for large Reynolds numbers up to $R=10^6$. The statistical quantities include skewness, entropy, dissipation energy, transfer functions, Taylor's micro-scale of both the velocity field and the concentration fields. These are presented in the form of graphs for the representative value of Reynolds number $R=10^6$. The analysis of the numerical values of statistical parameters thus obtained is carried out and the laws governing these quantities are investigated. Also, the merits and scope of the present closure scheme for studying similar types of turbulent flows are discussed.

Keywords: Turbulent mixing, Second order reactions, Factorised Cumulant Expansion Approximation Method, entropy, energy spectrum function, skewness, dissipation function, Taylor's micro-scale.

I. INTRODUCTION

Mixing is a phenomenon of multiple interests. In chemical industry in particular, mixing is of primordial importance for process control and optimization of chemical reactors. Many chemical reactions, either single – phase or multi-phase are of importance in both natural and industrial system, take place in turbulent flow fields. In general both the properties of the flow field in which the reaction occurs and the way the reactants are introduced in it will affect the spatial and temporal evolution of these systems. Further, the state of a particular system will be determined by the nature of the reaction kinetics involved and by the relative rates of the simultaneously occurring chemical and dispersion processes.

The state of environmental systems is turbulent for almost all common circumstances; on the other hand industrial flows and reaction systems are also deliberately, in most cases, in a turbulent state in order to utilize the enhanced rates of heat and mass transfer resulting from turbulent motions. (commonly called "turbulent mixing"). As a consequence, the problem of simultaneous turbulent mixing and chemical reaction is commonly encountered in a vast variety of different situations. The relevant research studies are conducted on problems arising in the fields such as chemical and environmental engineering, combustion and propulsion, aerodynamics, laser and plasma chemistry etc. The major interest today appears in the area of combustion research on turbulent combustion where the problem of interaction between reaction and turbulent mixing seems to assume its most complex level. Increasing interest has also been arising recently in various other fields, especially in environmental applications. More specifically, Donaldson and Hilst¹ (1972) and Lamb² (1973) recognized the importance of incomplete turbulent mixing phenomena in the processes of photochemical smog formation and number of related works have appeared since then. Due to both the variety of the problems in which the problem of reactive turbulence is encountered and wide range of approaches through which this problem is attacked, an attempt to get familiar with the essential of the entire spectrum of modeling techniques in the field would constitute a most difficult task. Basic aspects of such techniques are covered in standard textbooks in chemical engineering (Froment and Bischoff³ (1979) and in combustion theory (Williams⁴ (1985)). In particular the collection by Murthy⁵ (1975), Broadkey⁶ (1975) and Libby and Williams⁷ (1980), contains a wide range of applications from various fields and some excellent reviews of specific approaches. Among the review papers with a more general perspective, those of Hill⁸ (1976), which covers mainly the fluid – mechanical approach to the mixing-reaction problem and of Pratt⁹ (1979), which contains a brief summary of modern chemical reactor theory on the basis of population balance approaches, can serve as tutorial introduction to the subject of reactive turbulence. Some more recent developments not contained in the above works can be found in the works of

Villiermaux¹⁰(1983) and Pope¹¹ (1985), Joshi N.E. and Meshram M.C.¹²(1988), Meshram M.C. and Jhunjhare J.R.^{13,14}(2004), Meshram M.C.^{15,16}(2010,2012), Meshram M.C. and Sahu K.^{17,18} (2012) . Due to the rapid evolution of computing power over the last decades, numerical simulations have become an important domain of research in turbulence, which provides complementary information in addition to experiments.

As an attempt along this line, a FCEA method is proposed for the turbulence under study. A close set of equations for the energy spectrum functions are derived in Section 2. In section 3 the equations for energy spectrum functions are written in dimensionless form and then integrated numerically. The statistical quantities describing the turbulent reaction mixture with second order reaction such as energy, entropy, skewness, dissipation energy, transfer functions and Taylor’s micro-scales for concentration fields are evaluated from the numerical values of energy spectrum function of concentration fields. Thereafter, a detail analysis is carried out in section 4. The paper concludes with section 5 where the summary of the work is given and results obtained are discussed. In this section we also discuss the scope of the method for conducting further research.

II. EQUATIONS FOR THE ENERGY SPECTRUM FUNCTIONS

The theory of turbulence with reacting and mixing chemical elements with a second order irreversible, isothermic reactions may be developed in terms of joint probability distribution P in the space of the vector field $U(\mathbf{x}, t)$ and the n concentration scalar fields $A_p(\mathbf{x}, t)$, $p=1, 2, 3, \dots, n$, which satisfy the following system of equations:

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial P}{\partial x_i} + \gamma \frac{\partial^2 U_i}{\partial x_j \partial x_j} \quad (2.1a)$$

$$\frac{\partial A_p}{\partial t} + U_i \frac{\partial A_p}{\partial x_i} = D \frac{\partial^2 A_p}{\partial x_i \partial x_i} - K A_p A_q \quad (2.1b)$$

$$\nabla \cdot \mathbf{U} = 0 \quad (2.1c)$$

where $U = U(\mathbf{x}, t)$ = velocity of the flow field, $A_p = A_p(\mathbf{x}, t)$ = concentration of reactant p , D = molecular diffusivity, γ = kinematic viscosity and K = reaction rate.

In the present investigation we wish to develop a theory of turbulent multi-component reaction mixture with second order reactions in terms of a joint probability distribution P in the space of velocity vector field $U(\mathbf{x}, t)$ and the concentration scalar fields $A_p(\mathbf{x}, t)$ when the reaction is of the type $A+B \rightarrow \text{Product}$. In order to isolate the rate of small-scale fluctuation from other effects, the statistical homogeneity of the concentration fields A_p are assumed. Similarly, the turbulence is assumed to be isotropic, homogeneous and axisymmetric. We ignore the dynamic and chemical role of the product. To ensure simplicity, the reaction rate K is selected as constant and the stoichiometric coefficients q as unity. Even though the theory can be developed with these equations for n concentration fields, we restrict ourselves to two reactants A and B keeping future convenience in mind. Similar computations can be conducted for a practical study involving more than two reactants. Thus, for a turbulent mixture with reactants A and B , the system of simultaneous equations (2.1a), (2.1b) and (2.1c) is represented by following equations:

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial P}{\partial x_i} + \gamma \frac{\partial^2 U_i}{\partial x_j \partial x_j} \quad (2.2a)$$

$$\frac{\partial A}{\partial t} + U_i \frac{\partial A}{\partial x_i} = D_A \frac{\partial^2 A}{\partial x_i \partial x_i} - K A A \quad (2.2b)$$

$$\frac{\partial B}{\partial t} + U_i \frac{\partial B}{\partial x_i} = D_B \frac{\partial^2 B}{\partial x_i \partial x_i} - K B B \quad (2.2c)$$

$$\frac{\partial U_i}{\partial x_i} = 0 \quad (2.2d)$$

Here D_A and D_B represent the molecular diffusivity of reactant A and B respectively.

Repeated lower indices imply summation. The above equations are described in the work of O’Brien¹⁹ and Brodkey⁶.

M.C.Meshram and N.E. Joshi¹² defined the characteristic functional for the joint probability distribution of the velocity field and concentration fields P defined as follows

$$\Gamma[\bar{g}(\bar{x}, t); h_1(\bar{x}, t); \dots; h_\alpha(\bar{x}, t); \dots; h_n(\bar{x}, t)]$$

$$= \langle e^{i \int [\bar{g}(\bar{x}, t) \bar{U}(\bar{x}, t) + \sum_{\alpha=1}^n h_\alpha(\bar{x}, t) A_\alpha(\bar{x}, t)] d\bar{x} dt} \rangle \quad (2.3)$$

where $\bar{g}(\bar{x}, t)$ is arbitrary vector field and $h_\alpha(\bar{x}, t)$ are n number of scalar fields which vanish at spatial infinity; parenthesis $\langle \rangle$ indicates ensemble averaging over the entire space of velocity and concentration fields and bracket $[]$ represents the inner product of the vector fields. On using this characteristic functional they derived the functional differential equations for turbulence with the reacting and mixing elements of the type $A+B \rightarrow$ Product. Following A.S.Yaglom and A.M.Monin^{20, 21}; B. Szafirski²², Joshi N.E. and Meshram M.C.¹² defined the second characteristic functional $\psi\{\bar{y}(\bar{k}, t); \bar{z}_1(\bar{k}_1, t); \dots; \bar{z}_\alpha(\bar{k}_\alpha, t); \dots; \bar{z}_n(\bar{k}_n, t)\}$ as given below:

$$\Gamma[\bar{y}(\bar{k}, t); \bar{z}_1(\bar{k}_1, t); \dots; \bar{z}_\alpha(\bar{k}_\alpha, t); \dots; \bar{z}_n(\bar{k}_n, t)]$$

$$= \exp[\psi\{\bar{y}(\bar{k}, t); \bar{z}_1(\bar{k}_1, t); \dots; \bar{z}_\alpha(\bar{k}_\alpha, t); \dots; \bar{z}_n(\bar{k}_n, t)\}] \quad (2.4)$$

Where $\bar{y}(\bar{k}, t); \bar{z}_1(\bar{k}_1, t); \dots; \bar{z}_\alpha(\bar{k}_\alpha, t); \dots; \bar{z}_n(\bar{k}_n, t)$ are defined as

$$\bar{g}(\bar{x}, t) = \frac{1}{(2\pi)^3} \int \bar{y}(\bar{k}, t) e^{i\bar{k} \cdot \bar{x}} d\bar{k}$$

$$h_\alpha(\bar{x}, t) = \frac{1}{(2\pi)^3} \int z_\alpha(\bar{k}, t) e^{i\bar{k} \cdot \bar{x}} d\bar{k}$$

$$\alpha = 1, 2, \dots, n$$

They translated the equations in characteristic functional in terms of second characteristic functional and obtained the equations for the cumulants of various orders which describe dynamics of cumulants. The equations for cumulants thus obtained also reflect the characteristic difficulty of the turbulence theory. Thus, the characteristic difficulty of the turbulence problem has surfaced in the present investigation too and Prandtl²³ described such occurrence as the open problem of turbulence theory. Hence, we have to impose some assumptions to obtain a close set of equations for finite number of statistical cumulants. This is the also called closure problem in the statistical theory of turbulence. Although numerous studies for this problem have been proposed by many researchers, none of them seem to be successful to completely describe the phenomena under study. One such recent effort by T. Tatsumi, M. Yamada and T. Takei²⁴ is promising step in this direction. They have applied the FCEA method for the study of homogeneous turbulence. G.K. Batchelor²⁵ and S. Chandrasekhar²⁶ have shown that the phenomenological theory of turbulence in MHD can be developed to same extent as the corresponding theories in ordinary hydrodynamic turbulence. Hence we employed successfully the FCEA method for the study of the turbulent reaction mixture of the type $A+B \rightarrow$ Product. Having achieved the success in obtaining a close system of equations for cumulants in case of hydrodynamic and magnetohydrodynamic turbulence, we demonstrate below that a close system of cumulants can be obtained for the turbulent reaction mixture if FCEA method is applied.

By employing multiple-scale-cumulant-expansion (MSCE) method, N.E.Joshi and M.C.Meshram¹² successfully obtained a closed set of equations for cumulants and derived the following equations for energy spectrum density function of velocity field $\phi^V(k, t)$ and energy spectrum density function of the concentration field $\phi^A(k, t), \phi^B(k, t)$.

$$\left(\frac{\partial}{\partial t} + 2\gamma k^2\right)\phi^V(k, t) = 4\pi \int_{-\infty}^{\infty} dk' \int_{-1}^1 \frac{1 - e^{-\gamma(k^2 + k'^2 + k''^2)t}}{\gamma(k^2 + k'^2 + k''^2)} k k'^3 \left(\frac{k k'}{k''^2} + \mu\right) (1 - \mu^2) \times$$

$$\{(\phi^V(k', t) - \phi^V(k, t))\phi^V(k'', t)\} d\mu \quad (2.5)$$

$$\left(\frac{\partial}{\partial t} + D k^2\right)\phi^A(k, t) = 4\pi \int_{-\infty}^{\infty} dk' \int_{-1}^1 \frac{1 - e^{-D(k^2 + k'^2 + k''^2)t}}{D(k^2 + k'^2 + k''^2)} q^2 \{(\phi^V(k', t) + \phi^A(k, t))\phi^A(k'', t)\}$$

$$k k'^3 \left(\frac{k k'}{k''^2} + \mu\right) (1 - \mu^2) d\mu \quad (2.6)$$

$$\left(\frac{\partial}{\partial t} + D k^2\right)\phi^B(k, t) = 4\pi \int_{-\infty}^{\infty} dk' \int_{-1}^1 \frac{1 - e^{-D(k^2 + k'^2 + k''^2)t}}{D(k^2 + k'^2 + k''^2)} q^2 \{(\phi^V(k', t) + \phi^B(k, t))\phi^B(k'', t)\} k k'^3 \left(\frac{k k'}{k''^2} + \mu\right) (1 - \mu^2) d\mu$$

(2.7) Where

$$k''^2 = k^2 + k'^2 + 2\mu k k'$$

M.C. Meshram and K. Sahu^{17,18} successfully obtained positive energy spectrum function on employing this closure scheme and were successful in deriving various similarity laws governing the energy spectrum functions and other statistical quantities for Reynolds number as large as 10^6 . The relative success of the MSCE method has been appreciated by Taniuti²⁷ (1986). Fourth-order cumulant plays an important role in the dynamics of turbulence. Takayasu²⁸ (1985) and Kaneda²⁹ (1985) claimed that fourth order cumulant was not properly treated in the MSCE method. As a reply to this suggestion for proper handling of fourth order cumulant, T. Tatsumi, M. Yamada and T. Takei²⁴ introduced a FCEA method which amounts to expressing a n^{th} order cumulant $C^{(n)}$ as a fractional product of the cumulants $C^{(2)}$, $C^{(3)}$ and $C^{(n-1)}$.

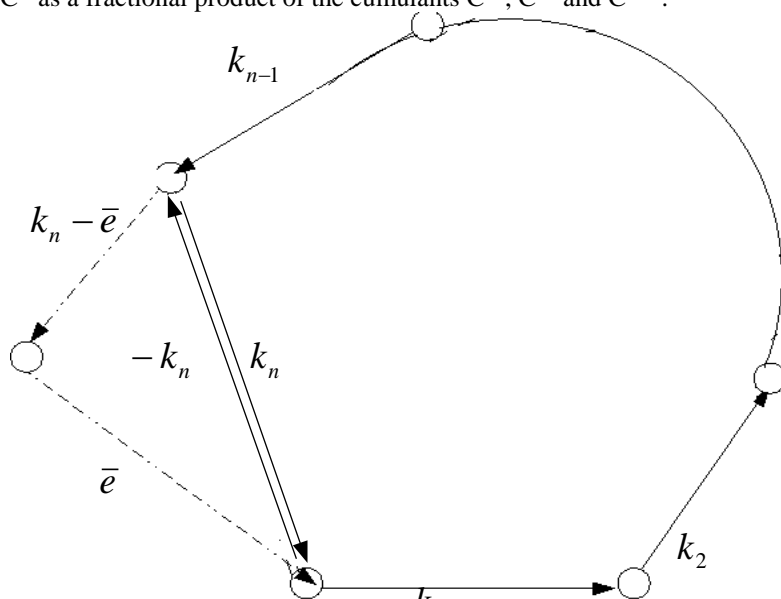


Figure 1 Polygon composed of $n+1$ wavenumber vectors

The $(n + 1)$ wavenumber vectors $(\bar{k}_1, \dots, \bar{k}_r, \bar{k}_{r+1}, \dots, \bar{k}_n, \bar{k}_n - \bar{e}, \bar{e})$, which are the arguments of the cumulant $\bar{C}^{(n+1)}$, compose a $(n+1)$ - polygon as depicted in above figure. Such a $(n+1)$ - polygon may be divided into two parts: a fixed n -polygon $(\bar{k}_1, \dots, \bar{k}_r, \bar{k}_{r+1}, \dots, \bar{k}_n)$ and a variable triangle $(-\bar{k}_n, \bar{k}_n - \bar{e}, \bar{e})$.

The cumulant $\bar{C}^{(n+1)}$ is expressed as a product of $C^{(n)}$ and $C^{(3)}$ as follows:

$$\bar{C}^{(n+1)} = \frac{\int C_{rpq}^{(3)}(-\bar{k}_n, \bar{k}_n - \bar{e}, \bar{e}; t) d\bar{e}}{\frac{1}{2} C_{ss}^{(2)}(\bar{k}_n, -\bar{k}_n; t)} C_{l_1 \dots l_{n-1} r}^{(n)}(\bar{k}_1, \dots, \bar{k}_{n-1}, \bar{k}_n; t) \quad (2.8)$$

where the division by $C^{(2)}$ has been made in order to maintain the equality of orders of the cumulants on both sides and the factor $\frac{1}{2}$ has been inserted so as to make the above relation an exact identity for the case $n = 2$. Following T. Tatsumi, M. Yamada and T. Takei²⁴ we employ factorised-cumulant-expansion-approximation method for the investigation of turbulence with reacting and mixing chemical elements of the type $A+B \rightarrow \text{Product}$ and obtain following equations (2.9), (2.10) and (2.11) for equations (2.5), (2.6) and (2.7):

$$\left(\frac{\partial}{\partial t} + 2\gamma k^2\right)\phi^V(k,t) = 4\pi \int_0^t dt' \int_0^\infty dk' \int_{-1}^1 \sqrt{\frac{\phi^V(k,t)\phi^V(k',t)\phi^V(k'',t)}{\phi^V(k,t')\phi^V(k',t')\phi^V(k'',t')}} k k'^3 \left(\frac{k k'}{k''^2} + \mu\right) (1 - \mu^2) (\phi^V(k',t') - \phi^V(k,t')) \phi^V(k'',t') d\mu \quad (2.9)$$

$$\left(\frac{\partial}{\partial t} + 2Dk^2\right)\phi^A(k,t) = 4\pi \int_0^t dt' \int_0^\infty dk' \int_{-1}^1 \sqrt{\frac{\phi^A(k,t)\phi^A(k',t)\phi^A(k'',t)}{\phi^A(k,t')\phi^A(k',t')\phi^A(k'',t')}} k k'^3 \left(\frac{k k'}{k''^2} + \mu\right) (1 - \mu^2) (\phi^V(k',t)\phi^A(k',t') + \phi^A(k,t')\phi^A(k,t')) d\mu \quad (2.10)$$

$$\left(\frac{\partial}{\partial t} + 2Dk^2\right)\phi^B(k,t) = 4\pi \int_0^t dt' \int_0^\infty dk' \int_{-1}^1 \sqrt{\frac{\phi^B(k,t)\phi^B(k',t)\phi^B(k'',t)}{\phi^B(k,t')\phi^B(k',t')\phi^B(k'',t')}} k k'^3 \left(\frac{k k'}{k''^2} + \mu\right) (1 - \mu^2) (\phi^V(k',t)\phi^B(k',t') + \phi^B(k,t')\phi^B(k,t')) d\mu \quad (2.11)$$

Equations (2.9) ,(2.10) and (2.11) describe the dynamics of the energy spectrum density function for the velocity field and concentration fields A and B respectively.

III. NUMERICAL CALCULATION

Defining the energy spectrum function $E(k,t)$ and the energy transfer function $T(k,t)$ in terms of energy spectrum density function as usual by

$$E(k,t) = 4\pi k^2 \phi(k,t) \quad (3.1)$$

$$T(k,t) = 4\pi k^2 \left(\frac{\partial}{\partial t} + 2\gamma k^2\right)\phi(k,t) \quad (3.2)$$

The equations (2.9) ,(2.10) and (2.11) for energy spectrum density functions $\phi^A(k,t)$ and $\phi^B(k,t)$ are expressed in terms of energy spectrum functions of concentration field A, $E^A(k,t)$ and concentration field B, $E^B(k,t)$ as follows:

$$\left(\frac{\partial}{\partial t} + 2\gamma k^2\right)E^V(k,t) = \int_0^t dt' \int_0^\infty dk' \int_{-1}^1 \sqrt{\frac{E^V(k,t)E^V(k',t)E^V(k'',t)}{E^V(k,t')E^V(k',t')E^V(k'',t')}} \frac{k k'}{k''^2} \left(\frac{k k'}{k''^2} + \mu\right) (1 - \mu^2) (k^2 E^V(k',t') - k'^2 E^V(k,t')) E^V(k'',t') dk' d\mu \quad (3.3)$$

$$\left(\frac{\partial}{\partial t} + 2Dk^2\right)E^A(k,t) = \int_0^t dt' \int_0^\infty dk' \int_{-1}^1 \sqrt{\frac{E^A(k,t)E^A(k',t)E^A(k'',t)}{E^A(k,t')E^A(k',t')E^A(k'',t')}} \frac{k k'}{k''^2} \left(\frac{k k'}{k''^2} + \mu\right) (1 - \mu^2) (k^2 E^V(k',t)E^A(k',t') + k'^2 E^A(k,t')E^A(k,t')) dk' d\mu \quad (3.4)$$

$$\left(\frac{\partial}{\partial t} + 2Dk^2\right)E^B(k,t) = \int_0^t dt' \int_0^\infty dk' \int_{-1}^1 \sqrt{\frac{E^B(k,t)E^B(k',t)E^B(k'',t)}{E^B(k,t')E^B(k',t')E^B(k'',t')}} \frac{k k'}{k''^2} \left(\frac{k k'}{k''^2} + \mu\right) (1 - \mu^2) (k^2 E^V(k',t)E^B(k',t') + k'^2 E^B(k,t')E^B(k,t')) dk' d\mu \quad (3.5)$$

We must emphasize that the present study relates to the investigation of turbulence with reacting and mixing chemical elements A and B. Here A and B are not chosen as any specific reactants as we wish to present the investigations in the general form. For the study of specific reactants their corresponding initial values for spectral density functions may be selected and the

investigation be carried out corresponding to those specific reactants. Also, for the present study we have selected Schmidt number Sc ($Sc = \frac{g}{D}$) as unity since not much information is lost by this assumption. The Schmidt number represents the ratio of the kinematic viscosity of the fluid and the molecular diffusivity of particular species. We have also assumed equal diffusivities for all species.

We numerically solve equations (3.3), (3.4) and (3.5) for energy spectrum functions under the following initial conditions:

$$E^V(k,0) = 4\pi E_0^V \frac{\left(\frac{k}{k_0}\right)^4}{\left[1 + \left(\frac{k}{k_0}\right)^8\right]} \quad (3.6a)$$

$$E^A(k,0) = 4\pi E_0^A \frac{\left(\frac{k}{k_0}\right)^4}{\left[1 + \left(\frac{k}{k_0}\right)^8\right]} \quad (3.6b)$$

$$E^B(k,0) = 4\pi E_0^B \frac{\left(\frac{k}{k_0}\right)^4}{\left[1 + \left(\frac{k}{k_0}\right)^8\right]} \quad (3.6c)$$

where E_0 and k_0 denote the representative values of the energy spectrum and the wavenumber respectively. The initial energy spectrum (3.6a), (3.6b) and (3.6c) has vanishing energy density $\frac{E^A(k,0)}{4\pi k^2}$ and $\frac{E^B(k,0)}{4\pi k^2}$ at zero wavenumber.

For the convenience of numerical work all variables are made nondimensional with respect to a representative wavenumber k_0 and a representative value of the energy spectrum E_0 and the solutions are expressed as functions of the nondimensional wavenumber, time and Reynolds number:

Wavenumber $\kappa = \frac{k}{k_0}$; Time $\tau = E_0^{\frac{1}{2}} k_0^{\frac{3}{2}} t$; Reynolds number $R = \frac{E_0^{\frac{1}{2}}}{\nu k_0^{\frac{1}{2}}}$

The equations (3.3), (3.4) and (3.5) in non-dimensional form are translated as follows

$$\left(\frac{\partial}{\partial \tau} + \frac{2}{R}\kappa^2\right)E^V(\kappa, \tau) = \int_0^\tau d\tau' \int_0^\infty \int_{-1}^1 \sqrt{\frac{E^V(\kappa, \tau)E^V(\kappa', \tau)E^V(\kappa'', \tau)}{E^V(\kappa, \tau')E^V(\kappa', \tau')E^V(\kappa'', \tau')}} \frac{\kappa\kappa'}{\kappa'^{1/2}} \left(\frac{\kappa\kappa'}{\kappa'^{1/2}} + \mu\right) (1 - \mu^2) \left(\kappa^2 E^V(\kappa', \tau') - \kappa'^2 E^V(\kappa, \tau')\right) E^V(\kappa'', \tau') d\kappa' d\mu \quad (3.7)$$

$$\left(\frac{\partial}{\partial \tau} + \frac{2}{R}\kappa^2\right)E^A(\kappa, \tau) = \int_0^\tau d\tau' \int_0^\infty \int_{-1}^1 \sqrt{\frac{E^A(\kappa, \tau)E^A(\kappa', \tau)E^A(\kappa'', \tau)}{E^A(\kappa, \tau')E^A(\kappa', \tau')E^A(\kappa'', \tau')}} \frac{\kappa\kappa'}{\kappa'^{1/2}} \left(\frac{\kappa\kappa'}{\kappa'^{1/2}} + \mu\right) (1 - \mu^2) \left(\kappa^2 E^V(\kappa', \tau)E^A(\kappa', \tau') + \kappa'^2 E^A(\kappa, \tau')E^A(\kappa, \tau')\right) d\kappa' d\mu \quad (3.8)$$

$$\left(\frac{\partial}{\partial \tau} + \frac{2}{R}\kappa^2\right)E^B(\kappa, \tau) = \int_0^\tau d\tau' \int_0^\infty \int_{-1}^1 \sqrt{\frac{E^B(\kappa, \tau)E^B(\kappa', \tau)E^B(\kappa'', \tau)}{E^B(\kappa, \tau')E^B(\kappa', \tau')E^B(\kappa'', \tau')}} \frac{\kappa\kappa'}{\kappa'^{1/2}} \left(\frac{\kappa\kappa'}{\kappa'^{1/2}} + \mu\right) (1 - \mu^2) \left(\kappa^2 E^V(\kappa', \tau)E^B(\kappa', \tau') + \kappa'^2 E^B(\kappa, \tau')E^B(\kappa, \tau')\right) d\kappa' d\mu \quad (3.9)$$

The numerical integration of eq. (3.8) and (3.9) is carried out for $R = 10^6$. The integration with respect to κ'' is made using the

trapezoidal sum rule with uneven mesh sizes $\kappa' = \frac{k'}{k_0} = ab^n$, $a = 0.1$, $b = 1.115$, $n = 1, 2, \dots, 70$ and the integration with respect to μ are made using the 40 point Legendre-Gauss method. The time integration is done by the forward difference method with the increment $\Delta\tau = 0.001$.

In the entire discussion below the energy spectrum function $E^V(k, t)$ shall not be discussed as all relations governing $E^V(k, t)$ are not different from those obtained by T. Tatsumi et.al.²⁴ and do not fetch any additional information for the velocity field.

IV. EVALUATION OF STATISTICAL QUANTITIES AND ANALYSIS

The equations (3.8) and (3.9) are solved numerically for the initial conditions (3.6b) and (3.6c); the Reynolds number $R=10^6$; and the energy spectrum functions $E^V(k, t)$, $E^A(k, t)$ and $E^B(k, t)$ are obtained as functions of the wavenumber k and time t . Of all the numerical data concerning the evolution of energy spectrum function of concentration field $E^A(k, t)$ and energy spectrum function of concentration field B, $E^B(k, t)$ respectively for $R=10^6$ are shown graphically in figure 4.1. We observe that the forms of these functions, especially those at higher wavenumbers, are displayed more clearly on a logarithmic scale. Hence, we have used the logarithmic scales for plotting of the graphs representing the behaviour of various statistical quantities under study.

The general appearance of the energy spectrum function is similar to that obtained on using modified-zero-fourth-cumulant-expansion- approximation (MZFCEA) method. Both the energy spectrum function $E^A(k, t)$ and magnetic energy spectrum function $E^B(k, t)$ are found to be positive definite at all times for Reynolds numbers as large as 10^6 .

It may be seen that the functions $E^A(k, t)$, $E^B(k, t)$ and $T^A(k, t)$, $T^B(k, t)$ undergo rapid change in an initial stage which extends from $\tau = 0$ to about $\tau = 3$ and thenceforth change rather slowly and similarly in time. The general trend of the change in the spectrum functions $E^A(k, t)$, $E^B(k, t)$ are analogous with those observed in case of the MZFCEA method. At very small wavenumbers below the energy-containing wavenumber roughly corresponding to $\kappa \cong 1 (k \cong k_0)$, the spectrum takes the form,

$$E^A(k, t) = A^A(t)k^{2.52} \tag{4.1a}$$

$$E^B(k, t) = A^B(t)k^{2.68} \tag{4.1b}$$

for $k \cong 0$ with a slowly increasing functions in time $A^A(t)$ and $A^B(t)$. G.K. Batchelor and I. Proudman²⁹ have obtained the variance of the coefficient A(t) for general homogeneous turbulence. In present investigation we notice that the coefficients $A^A(t)$ and $A^B(t)$ are not identical and take nearly equal values with time. We observe that the laws stated in (4.1a) and (4.1b) above are as per expectation for turbulent reaction mixture. In the energy-containing wavenumber range around $\kappa \cong 1 (k \cong k_0)$, the spectrum $E^A(k, t)$ and $E^B(k, t)$ do not seem to satisfy any similarity law. This behaviour of the energy spectrum functions is different from that due to the MZFCEA method and may be accounted to the fact that, unlike the counterpart of the latter approximation, the integrand on the right-hand side of equations (3.4) and (3.5) has two time variables t and t' .

An eminent feature of the present result is that there exists an extensive wavenumber range, in which the spectrum takes the form,

$$E^A(k, t) \propto k^{-2.3} \tag{4.2a}$$

$$E^B(k, t) \propto k^{-2.5} \tag{4.2b}$$

and satisfies a similarity laws. On the other hand, the present result has no k^{-1} range which existed next to the k^{-2} . Such coincidence and discrepancy of the spectrum forms in the present and the latter approximations may be attributed to the closeness and difference of the energy transfer integrals due to the two approximations.

At very large wavenumbers beyond the k^{-2} range, the spectrum shows exponential decay which may be expressed as

$$E^A(k, t) \propto \exp(-b^A k) \tag{4.3a}$$

$$E^B(k, t) \propto \exp(-b^B k) \tag{4.3b}$$

for $k \rightarrow \infty$, with positive constants b^A and b^B . Such an asymptotic behaviour of the spectrum was also predicted by the MZFCEA method. This asymptotic behaviour is in fact due to an asymptotic form of the right-hand side of equations (3.4) and (3.5). Thus, the spectrum functions in the very low wavenumber range are entirely fixed by the initial conditions, reflecting the well known permanence of the large scale component of turbulence.

The entropy of the concentration field A, $\varepsilon^A(t)$ and entropy of the concentration field B, $\varepsilon^B(t)$ are respectively given by

$$\varepsilon^A(t) = 4\pi \int_0^\infty k^2 \phi^A(k, t) dk \tag{4.4a}$$

$$\varepsilon^B(t) = 4\pi \int_0^\infty k^2 \phi^B(k, t) dk \tag{4.4b}$$

These quantities mostly reflect the shape of energy spectrum functions $E^A(k, t)$ and $E^B(k, t)$ in the energy containing range of the wavenumber. Entropy of the concentration field A and concentration field B is defined by the integrals (4.4a) and (4.4b). The equations (3.7) and (3.8) are integrated numerically and obtained the numerical values of the energy spectrum function of both concentration field A and concentration field B. The values of energy spectrum functions thus obtained are used to find the numerical values of entropy of the concentration field A and concentration field B and the plots of these values are shown in figure 4.2. We infer from these graphs of entropy of the concentration field A and concentration field B that they are analogous to each other. The entropy of both the concentration field A and concentration field B grows very rapidly in the initial stage, attains a quite large maximum value at about $\tau = 1$, and decays nearly similarly in the later period. The decay laws are given as

$$\varepsilon^A(t) \propto t^{-2.45} \tag{4.5a}$$

$$\varepsilon^B(t) \propto t^{-2.52} \tag{4.5b}$$

which are compatible with the energy decay laws and agree quite well with the established findings. The comparison of the decay of entropy functions indicate that entropy of concentration field A decay faster than that and concentration field B.

The Skewness of and concentration field A, $S^A(t)$ and that of concentration field $S^B(t)$ is respectively defined by equations (4.6a) and (4.6b) below:

$$S^A(t) = \frac{3\sqrt{30}}{14} \frac{5 \int_0^\infty k^2 T^A(k, t) dk}{\left[\int_0^\infty k^2 E^B(k, t) dk \right]^{3/2}} \tag{4.6a}$$

$$S^B(t) = \frac{3\sqrt{30}}{14} \frac{5 \int_0^\infty k^2 T^B(k, t) dk}{\left[\int_0^\infty k^2 E^B(k, t) dk \right]^{3/2}} \tag{4.6b}$$

The equations (3.8) and (3.9) are integrated numerically and obtained the numerical values of the energy spectrum function for the concentration field A and energy spectrum function of the concentration field B. The values of energy spectrum functions thus obtained are used to find the numerical values of skewness of the concentration field A and concentration field B. Figure 4.3 depicts the skewness of both the fields for different values of time. We infer from this graph of skewness for concentration field A and concentration field B that their behaviour is analogous to each other. We also notice from this graph that the initial values of both the skewness are very close to one. The complete curve is divided into three parts. In the first part the magnitude of the skewness increases monotonically with time and concentration field A attains a maximum value of about 0.3 whereas concentration field B attains a value of maximum magnitude 0.8. In the intermediate parts both the fields decrease exponentially in a similar fashion and in the final part growth of skewness of both the fields is quadratic. Such a behaviour of the skewness largely diverges from the previous results including those derived from the MZFCEA method by M.C Meshram and K. Sahu^{17,18}.

.At the moment it is not certain if the magnitude of $S^A(t)$ and $S^B(t)$ would reduce drastically to a small stationary value

afterwards as was the case in the above-mentioned approximation or if the calculated values themselves would not be reliable due to the possible inaccuracy of the functions $E^A(k, t)$, $E^B(k, t)$ and $T^A(k, t)$, $T^B(k, t)$ at large wavenumbers. The predictions of the present closure scheme are in good agreement with the curves at the quasi-stationary state which guarantees the self-consistency of the numerical results.

The energy dissipation functions for velocity field and magnetic field respectively are defined by

$$D^A(k, t) = 2\nu k^2 E^A(k, t) \tag{4.7a}$$

$$D^B(k, t) = 2\nu k^2 E^B(k, t) \tag{4.7b}$$

The energy dissipation functions for concentration field A, $D^A(k, t)$ and concentration field B, $D^B(k, t)$ for $R=10^6$ are shown in figure 4.4. The energy spectrum function for concentration field A dissipates quickly as compared to the energy spectrum function concentration field B.

The energy transfer function of concentration field A, $T^A(k, t)$ and energy transfer function for concentration field B, $T^B(k, t)$ respectively those for $R=10^6$ are shown graphically in figure 4.5. We notice from this figure that the trend of the growth of transfer spectra of concentration field A and concentration field B is different. Transfer functions of the concentration field A increase steadily and attain maximum values 4. After attaining these maximum values they show the decreasing trend indicating that an inverse transfer of energy of concentration field A is occurring at low wavenumber whereas transfer functions of the concentration field B first decreases then increases and attain maximum value of 17. The wavenumber at which transfer function vanish for the first time is different for both the concentration field A and concentration field B as against the result of earlier closure scheme wherein both the transfer functions vanished at same wavenumber.

For a given Reynolds number, in the neighbourhood of the wavenumber both the energy transfer functions change their sign satisfying the condition

$$\int_0^{\infty} T^A(k, t) dk = 0 \tag{4.8a}$$

$$\int_0^{\infty} T^B(k, t) dk = 0 \tag{4.8b}$$

as per the present closure scheme employed.

The Taylor's micro-scale for the concentration field A, $\lambda^A(t)$ and for the concentration field B, $\lambda^B(t)$ are defined and expressed in terms of the energy spectrum functions as given below:

$$\lambda^A(t) = \frac{5 \int_0^{\infty} E^A(k, t) dk}{\int_0^{\infty} k^2 E^A(k, t) dk} \tag{4.9a}$$

$$\lambda^B(t) = \frac{5 \int_0^{\infty} E^B(k, t) dk}{\int_0^{\infty} k^2 E^B(k, t) dk} \tag{4.9b}$$

The values of Taylor's micro-scale of the concentration field A, $\lambda^A(t)$ and for the concentration field B, $\lambda^B(t)$ are obtained by substituting numerical values of $E^A(k, t)$ and $E^B(k, t)$ into (4.9a) and (4.9b) and the numerical values thus obtained are plotted in figure 4.6 for Reynolds number $R=10^6$. The Taylor's microscale defined by (4.9a) and (4.9b) gives another parameter representing the small scale structure of turbulence with reacting and mixing chemical elements. For Reynolds numbers $R=10^6$ the micro-scale for the concentration field A and the concentration field B decrease very rapidly in the initial stage and then increases parabolically. The Taylor's micro-scale of the concentration field A, $\lambda^A(t)$ and that of the concentration field B, $\lambda^B(t)$ attain a minimum around $t=2.2$ and $t=2.1$ for $R=10^6$ respectively.

In the initial period the decrease in Taylor's micro-scale of the concentration field A, $\lambda^A(t)$ and that of the concentration field B, $\lambda^B(t)$ with time is governed by the laws that the micro-scale of both the fields varies proportionally to negative 0.4 power of the time. Symbolically these laws are represented as:

$$\lambda^A(t) \propto t^{-0.4} \tag{4.10a}$$

$$\lambda^B(t) \propto t^{-0.4} \tag{4.10b}$$

This variation of the Taylor’s micro-scale of concentration field **A** and that of the concentration field **B** with time confirms the asymptotic decrease of Taylor’s micro-scale with time.

Similarly in the final period the growth of the Taylor’s micro-scale of concentration field **A** and that of the concentration field **B** with time is governed by the laws that the micro-scale of both the fields varies proportionally to 0.8 power of the time. Symbolically these laws can be written as:

$$\lambda^A(t) \propto t^{0.8} \tag{4.11a}$$

$$\lambda^B(t) \propto t^{0.8} \tag{4.11b}$$

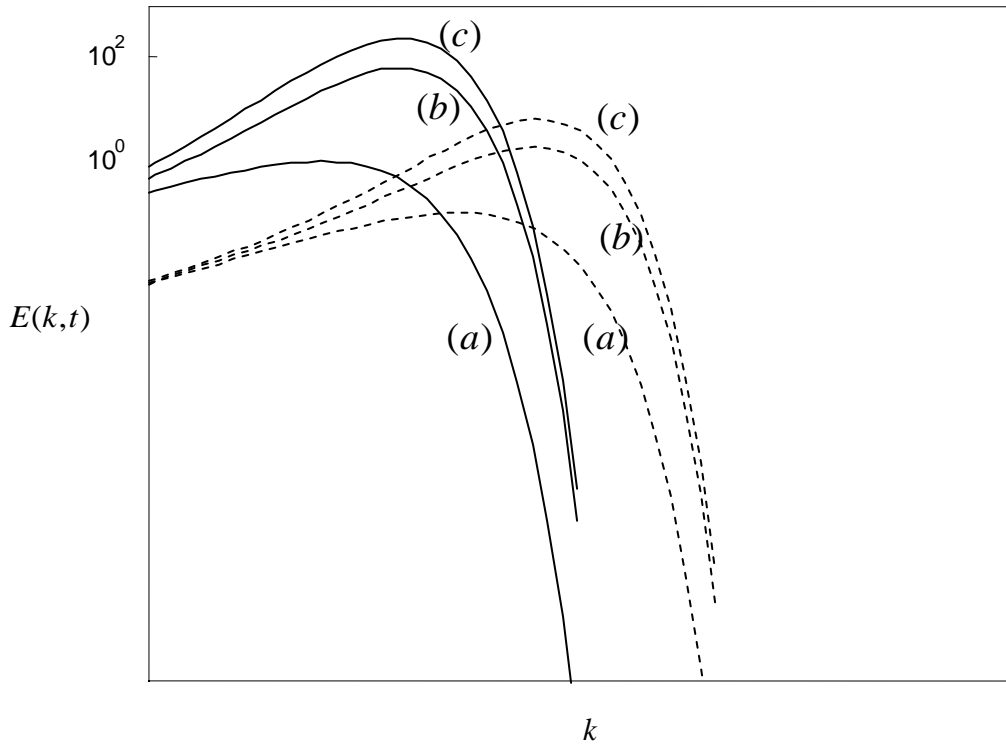


Figure 4.1 Energy spectrum function for concentration field **A** (solid lines) an concentration field **B** (dashed lines) for $R=10^6$ at (a) $t = 0$ (b) $t = 2$ and (c) $t = 4$

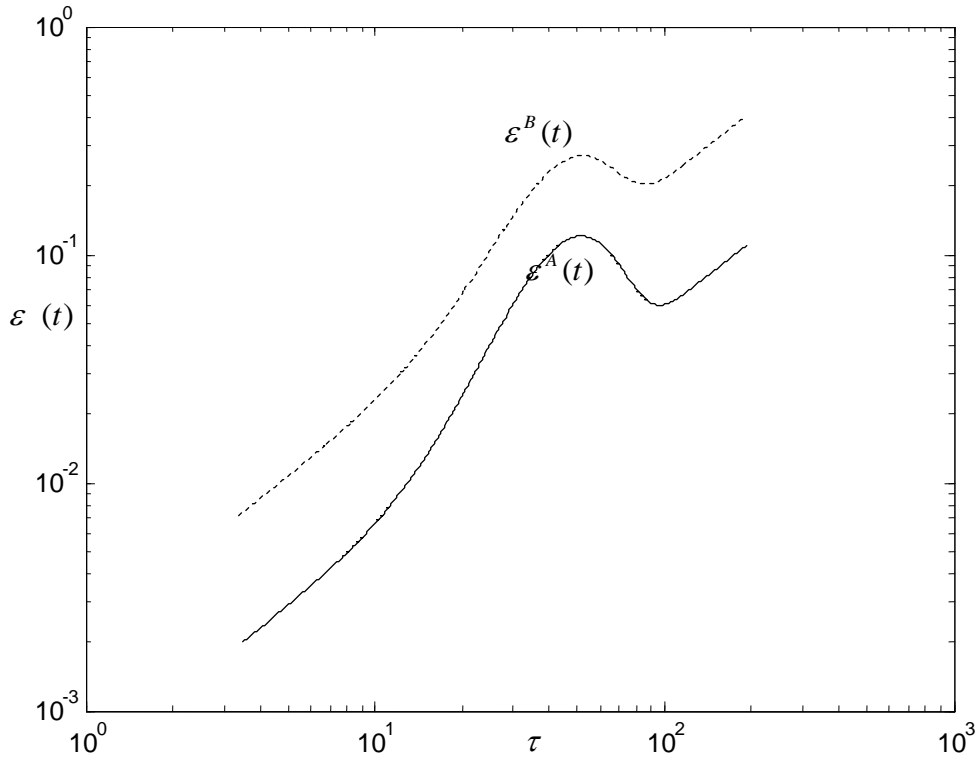


Figure 4.2 Enstrophy of the concentration field A (solid lines) and concentration field B (dashed lines) for Reynolds number $R=10^6$

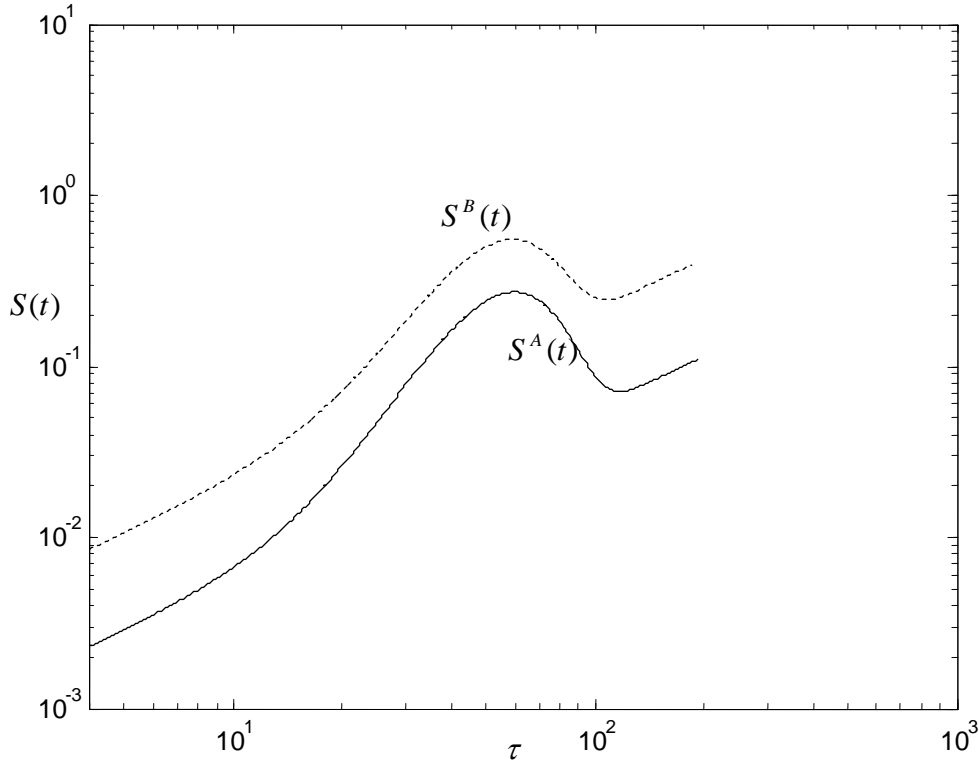


Figure 4.3 Skewness of the concentration field A (solid lines) and concentration field B (dashed lines) for Reynolds number $R=10^6$

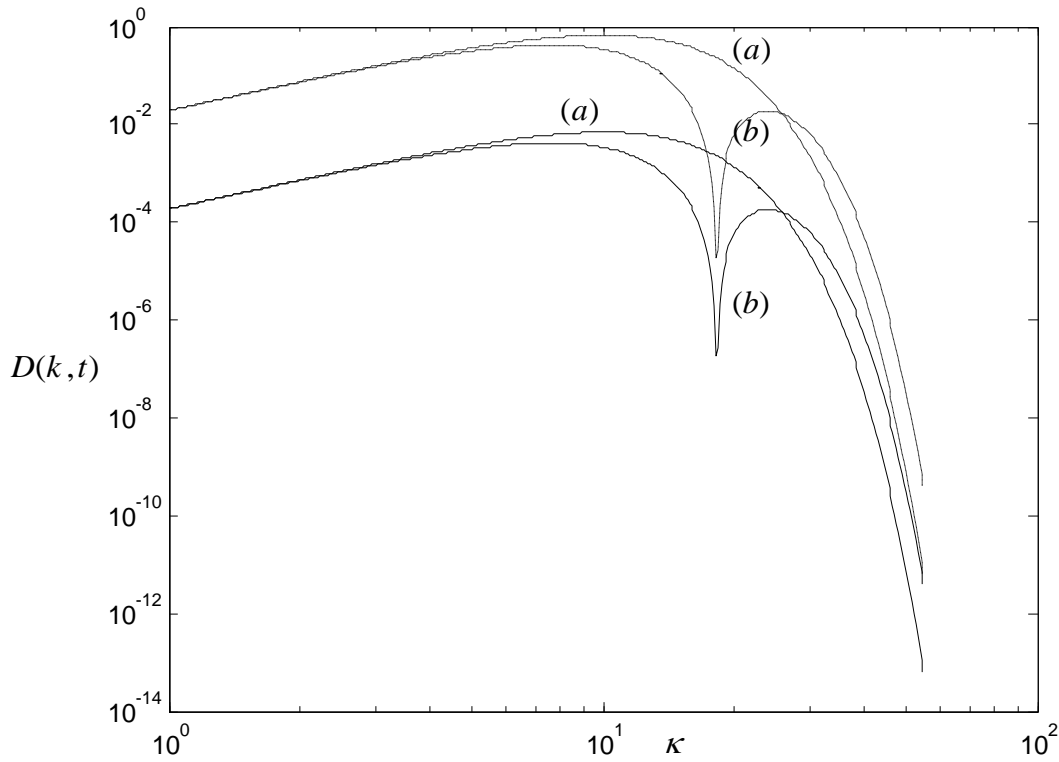


Figure 4.4 Energy dissipation function of the concentration field A (solid lines) an concentration field B (dashed lines) for Reynold number $R=10^6$ at (a) $t = 0$ and (b) $t = 3$

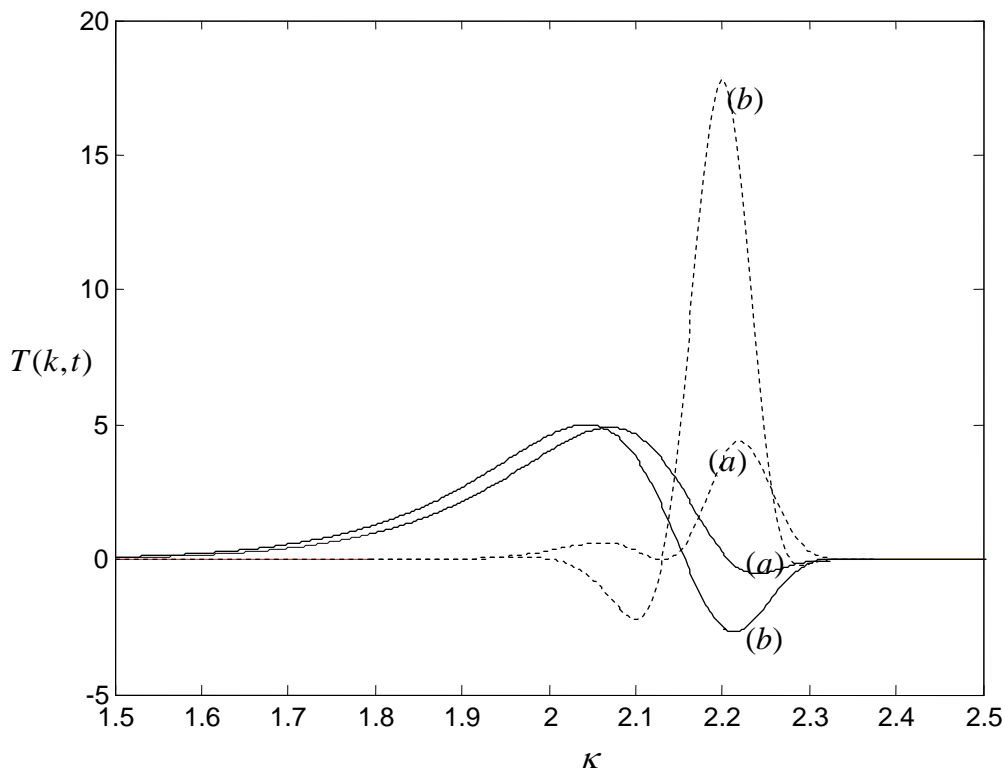


Figure 4.5 Energy transfer function of concentration field A (solid lines) an concentration field B (dashed lines) for Reynold number $R=10^6$ at (a) $t=0$ and (b) $t=3$

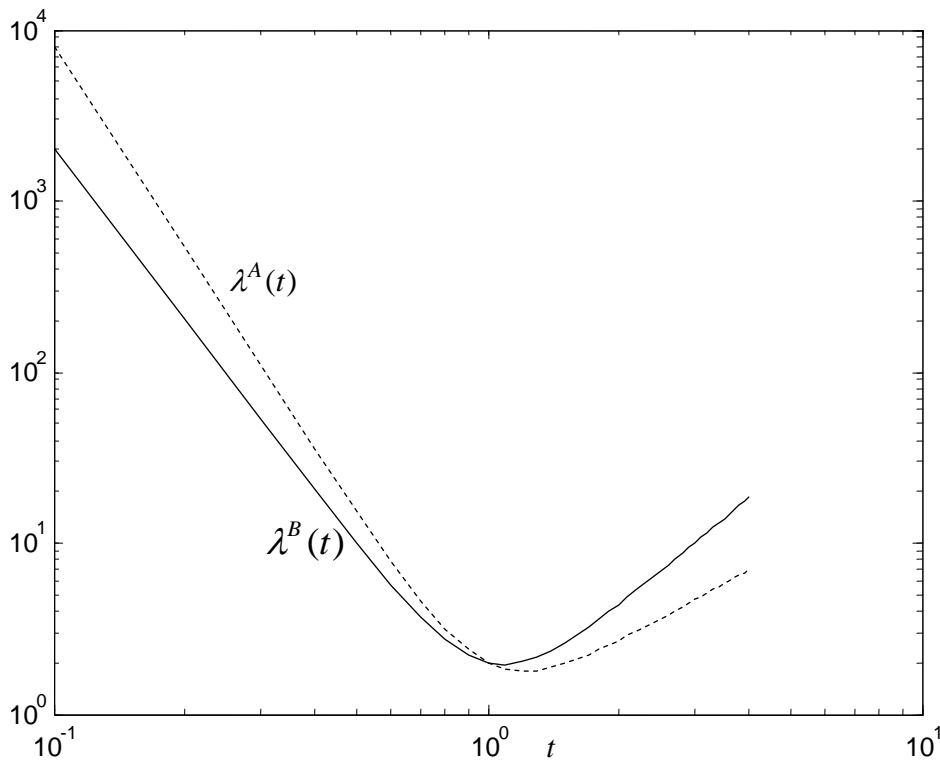


Figure 4.6 Taylor’s Micro-Scale of the concentration field A (solid line) and the concentration field B(dashed line) for Reynold number $R=10^6$

V. SUMMARY AND DISCUSSION

Turbulence with reacting and mixing chemical elements of the type $A+B \rightarrow \text{Product}$ is investigated statistically by employing Factorised –Cumulant-Expansion-Approximation method. The main results from this study can be summarized as follows.

1. The energy spectrum function of concentration field A, $E^A(k,t)$ and concentration field A, $E^B(k,t)$ are found to be positive definite at all times for Reynolds numbers as large as 10^6 .
2. The general trend of the change in both the spectrum functions is analogous with those observed in case of the modified-zero-fourth-cumulant-expansion-approximation method.
3. An eminent feature of the present result is that there exists an extensive wavenumber range, in which the spectrum takes the form,

$$E^A(k,t) \propto k^{-2.3}$$

$$E^B(k,t) \propto k^{-2.5}$$

4. The entropy of the concentration field A and that of concentration field B are analogous to each other.
5. The comparison of the decay of entropy functions indicate that entropy of concentration field B decay faster than that of concentration field A.
6. The behaviour of the skewness of concentration field A and concentration field B is analogous to each other.
7. The initial values of skewness of both the fields are very close to one.
8. The complete curve of the skewness of both the field is divided into three parts. In the first part the magnitude of the skewness increases monotonically with time and concentration field A attains a maximum value of about 0.3 whereas concentration field B attains a value of maximum magnitude 0.8. In the intermediate parts both the fields decreases exponentially in a similar fashion and in the final part a sudden quadratic growth is seen in skewness of both the fields.
9. The growth of transfer spectra of concentration field A and concentration field B is totally different. The transfer spectra for concentration field B increases steadily and attain maximum values 4 and 17 respectively at $t=0$ and $t=3$ whereas the transfer spectra of concentration field A increases and attain nearly the same maximum value at $t=0$ and $t=3$.
10. The micro-scale for the concentration field A and concentration field B decrease very rapidly in the initial stage and then increase is along a parabola.

11. For $R=10^6$ the Taylor's micro-scale of concentration field A, $\lambda^A(t)$ and that of the concentration field B, $\lambda^B(t)$ attain a minimum around $t=2.2$ and $t=2.1$ respectively.

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