行政院國家科學委員會補助專題研究計畫成果報告

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計畫主持人：洪祖昌

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行政院國家科學委員會專題研究計畫成果報告

紊流反應流之機率密度函數模式研究

THE PROBABILITY DENSITY FUNCTION APPROACH TO THE MODELING OF TURBULENT REACTING FLOWS

計畫編號：NSC 90-2212-E-032-005
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一、中文摘要

本計劃分為兩個相關部分。第一部份擬將洪等人所發展之速度紊流 pdf 模式加以擴展為可模擬具化學反應之紊流反應流之 pdf 模式，此新模式之獨立變數除了時間、空間及速度外，也包含標度(scalar)空間。模式化(modeling)過程將結合 Chung 與 Pope 之方法，並利用現象論雷諾應力模式之推導技巧，將影響紊流之各效應分別模式化，引入至模式中。第二部分將用此模式來預測擴散火焰。數值方法擬用 Monte Carlo 法及 Bimodal 法 。
關鍵詞：紊流、pdf 模式、擴散火焰

1. Abstract

This project includes two parts. The fist part is to extend the probability density function (pdf) turbulence model developed by Hong et al. to a new pdf model which can describe the turbulent fluid elements containing the chemically reactive species. The examination of the pdf model, the second part of this project, will be performed in predicting the diffusion methane jet flames. The Monte Carlo method will be used to calculate the pdf of the diffusion flame and the one-point statistical quantities of diffusion flame will be constructed.

Keywords: turbulence、pdf turbulence model、diffusion methane jet flames

2. Introduction

Turbulence is the most common, the most important and the most complicated kind of fluid motion [1]. The traditional solution is the phenomenological approach, directly modeling the high-order correlations in terms of the lower-order ones and determining the model constants with the aid of experimental data and mathematical analysis. This approach has some models such as two-equation and Reynolds-stress equation models [2-4]. An alternative approach, probability density function (pdf) methods, has been found to properly explain the featured turbulence structures due to the emphasis of probability density. Apart from being a solution for the pure turbulence field, the pdf methods are promising in the resolution of the turbulence issues complicated with chemical reactions. Over the last 20 years, a representative series of documents associated with pdf turbulence models have been published by Pope et al. [5-9].

In practice, the pdf turbulence models cannot be solved using conventional grid-based numerical methods because of their high dimensionality. This problem has been overcome using the Monte Carlo method developed by Pope [10]. Haworth and Pope [8] reported that every pdf turbulence model corresponded with a Reynolds-stress model (RSM). Furthermore, Pope [11] performed a detailed examination of the relationship between pdf models and RSMs. Because they are one-point closures, pdf models require external specification of scale information. To remedy this deficiency,

Pope and Chen [9] developed a pdf turbulence model based on the joint pdf of velocity and the instantaneous dissipation rate. Meanwhile, by combining the modeling methods of Chung [12] and Pope [5], Hong et al. developed a pdf model [13]. As compared with Pope's model [8-9], Hong et al.'s pdf model [13] is less complicated and includes viscous diffusion to deal with turbulence in the vicinity of a wall. Recently, Dreeben and Pops [14-15] also have included wall effects in their pdf models. Hong et al., subsequently, used their pdf model to predict the turbulent Couette flow [16] and the self-similar free shear layer flows [17-19].

It is well known that the conventional phenomenological approaches to turbulent shear flow chemical reaction problems have been developed to near their maximum capacities. These approaches have been very useful in analyzing non-equilibrium chemical reactions in various turbulent flow fields, in the absence of a more tractable method. It is known, however, that the correct description of a non-equilibrium chemical reaction in a turbulent flow field is outside the inherent limitations of the conventional phenomenological theories. Basically, it is because the rate of the chemical reaction in a turbulent flow field is coupled with the turbulent fluctuations so that the average chemical reaction rate at a given point is not equal to the rate based on the averaged properties, such as the averaged chemical species concentrations. As mentioned previously, pdf methods [7,9,12,13] can provide more statistical information than that provided by the conventional phenomenological models. This feature is attributed to the fact that once pdf is determined, any order mean can be constructed from the pdf. In addition, the pdf approach offers another advantage over the conventional phenomenological models: any one-point process such as convection, buoyancy and reaction can be treated without approximation. A thorough introduction to the pdf approach may be found in Ref. 1.

There are two major categories for which a pdf model equation is proposed for turbulent flows. One is to model those terms having additional dependent variables, such as f_2, which causes the closure problem in Lundgren's equation, in terms of known dependent variables, such as f_1, and other mean quantities (f_1 and f_2 represent the one point pdf and two point pdf, respectively). The typical closed pdf equation of this category can be found in Lundgren's [20], Pope's [5], and Dopazo's [21] works. Lundgren adopted the Krook model of molecular kinetic theory to approach the pressure term and assumed the two-point distribution is joint normal in his one-point pdf equation. It is widely accepted that turbulence fields evolve toward the dynamical state independent of the initial conditions of the velocity fields. Lundgren showed that the initial shape of the pdf is preserved in his closed pdf equation and, therefore, no relaxation was achieved. In Pope's work, the Curl's model was employed to simulate the viscous mixing which can produce an unrealistic shape for the pdf and does not lead to a Gaussian distribution as the limit of decaying fluctuations. Dopazo investigated the possibility of using a classical iteration method to generate a von Numann series for the pdf equation and thereby put some order into the closure approximations. The results are formal but not encouraging since the lowest terms in the approximation introduce unphysical features such as negative diffusivity. The modeling process for this category is straightforward, and the relations between the modeled results and unclosed terms are clear. The physical behavior of these terms are also distinct. As one can see from the above investigations, those models were proposed directly on the distribution function. It is hard to prevent generating unphysical behaviors in the distribution function. This is the major shortcoming of this category.

Chung's theory [12] is a typical work of the other category [6,8,12,22]. Chung avoided the closure problem using a thoroughly different approach. He assumed that the statistical property of a fluid element is entirely due to the lower non-equilibrium wave-number, and that the role of the higher equilibrium wave-number is to degenerate to a random state and dissipate this property by their interaction with lower wave-numbers.

When the Reynolds number is sufficiently large, a statistical separation exists between the higher and lower wave-numbers across an inertial sub-range. The dynamics of various wave-numbers in turbulence fields can be seen as closely related to Prigogine's description [23] of generalized Brownian motion. Thus Chung employed Langevin's stochastic equation of the generalized Brownian motion to describe the momentum change of a fluid element under the interaction of large and small size eddies at high Reynolds number flow. Then a transition pdf (tpdf) between two neighboring points in the phase space connected by the path of the fluid elements was constructed from the solution of the stochastic Langevin equation with the aid of Chandrasekhar's mathematical lemma [24] in Brownian motion. Finally Chung obtained a closed pdf equation by unfolding the tpdf in the phase space. It is worthwhile to mention that Chung used Langevin equation to describe the dynamic behavior of fluid elements to avoid the closure problem and introduced a characteristic relaxation rate to make this equation self-contained. It is newly introduced relaxation rate, β, the turbulent scale has to be prescribed. In Chung's work the Langevin equation was employed to propose a model for describing the fluid element dynamics. The pdf transport equation was then obtained based on the modeled dynamic equation of fluid elements. As mentioned by Chung himself that his equation could be seen as a Fokker-Planck type for Lundgren's pdf equation.

Pope proposed a generalized Langevin equation [6] to describe fluid element behaviors in a turbulent field. In his work, the generalized Langevin equation was just rewritten from the Navier-Stokes equation by analogy to the Langevin equation of Brownian motion. Obviously, this was based on the assumption that the Langevin equation, originally proposed to describe the Brownian motion of small particles resulting from collisions with Gaseous or liquid molecules, can be used to describe turbulent flows. Haworth and Pope [8,22] used this generalized Langevin equation to construct their generalized Langevin pdf model. The major difference between Haworth & Pope's model and Chung's model is that the characteristic relaxation rate of energy containing eddies, β, of Chung's model was replaced by a more flexible, undetermined 2nd order tensor G_{ij}. With different choices for G_{ij}, the Reynolds-stress equations degenerated from Haworth and Pope's model can be fitted to a variety of existing Reynolds-stress models. However, the above models can provide no information on length and time scales. To remedy this deficiency, Pope and Chen [9] recently developed a model based on the joint pdf of velocity and the instantaneous dissipation rate. This model was developed by reference to the known statistics of homogeneous turbulence, and in its original form it is restricted to homogeneous turbulence. Subsequently, Pope [25] extended the model to the general case of inhomogeneous flows, and calculations were made to demonstrate its performance. The major advantage of this approach is that no assumption was specified for pdf, therefore the unphysical behavior of pdf would not appear.

In this paper, the methods of the above two categories are employed to construct a new closed pdf equation for turbulent reactive flows [26]. First, the stochastic dynamics of a fluid element in turbulence fields is assumed to be a Markov process. At high Reynolds number flows, the fluctuating momentum change due to viscous force is controlled by the properties of large scale eddies. The fluctuating pressure forces acting on a fluid element are simulated by a Wiener process. The governing equation of fluid element velocity fluctuations are obtained from the fluctuation part of the Navier-Stokes equation. The fluctuation part of the stress-strain relation are reformulated under the above assumptions such that the length scale information is represented by the turbulent dissipation rate. The moment equations derived from the pdf equation are compared with the accurate and proven Reynolds stress model equation [27-30] to determine the modeling constants. Through this process, it is expected that the final pdf model can properly describe the pdf behavior of turbulent reactive flows.

3. Result

Auxiliary Mathematical Lemma

In this subsection, Chandrasekhar's lemma [24], which can construct the tpdf of two neighboring points in the phase space in Brownian motion theory, was extended to be employed later in this work to construct the tpdf. The auxiliary mathematical lemma is stated as follows. Let R be a random variable, $R=R_1 i+R_2 j+R_3 k$ can be expressed as

$$R_i = \int \varphi_i(\varsigma) A(\varsigma) d\varsigma \quad (1)$$

where A(ζ) is a Wiener process with a Gaussian distribution, φ(ζ) are any auxiliary functions. And R_1, R_2, and R_3 are independent of each other. Then the probability distribution of R is

$$W(R_1,R_2,R_3) = \left[4\pi q\int_0^t \varphi_1^2(\varsigma)d\varsigma\right]^{-0.5}\left[4\pi q\int_0^t \varphi_2^2(\varsigma)d\varsigma\right]^{-0.5} \times\left[4\pi q\int_0^t \varphi_3^2(\varsigma)d\varsigma\right]^{-0.5} \bullet \exp\left[\frac{-R_1^2}{4q\int_0^t \varphi_1^2(\varsigma)d\varsigma}+\frac{-R_2^2}{4q\int_0^t \varphi_2^2(\varsigma)d\varsigma}+\frac{-R_3^2}{4q\int_0^t \varphi_3^2(\varsigma)d\varsigma}\right] \quad (2)$$

Details about this auxiliary lemma are given in Ref. 31.

PDF Transport Equation

In this subsection, the processes in deriving and modeling the transport equation for the one-point velocity pdf of a reactive turbulent are described in great detail. For turbulent flow, the instantaneous velocity can be decomposed into mean and fluctuation parts as, $u_i=\langle u_i\rangle+U_i$, where u_i, $\langle u_i\rangle$, and U_i are the instantaneous, mean, and fluctuating velocities, respectively. Then the dynamic equation governing the change of fluctuating momentum of a fluid element can be obtained by subtracting the Reynolds average equation from the Navier-Stokes equation

$$\frac{dU_i}{dt} = -\frac{\partial \langle u_i\rangle}{\partial X_j}U_j + \frac{\partial \langle U_i U_j\rangle}{\partial X_j} - \frac{1}{\rho}\frac{\partial P}{\partial X_i} + \nu\frac{\partial^2 U_i}{\partial X_j^2}. \quad (3)$$

where d/dt denotes the instantaneous substantial derivative, P the fluctuating pressure, ρ and ν for density and kinematic viscosity, respectively, and the angle brackets represent an ensemble mean. The last two terms in the right-hand side of Eq. (3) represent the pressure force and viscous force acting on the fluid elements, respectively. These two terms lead towards the unavoidable closure problem in the pdf equation of Lundgren. These two terms are contributed mainly by the small eddies (high frequency). If the details regarding the dynamics of the smallest eddies are not desired, the smallest eddies can be generally regarded as being both very numerous and also very irregular as to their strength and direction. A turbulent flow should consequently be treated as a stochastic process and the pressure force and viscous force terms in Eq. (3) should be modeled.

The major effect of molecular viscosity in turbulent flows lies in dissipate turbulent energy. Additionally, the amount of energy dissipated at higher wave-numbers is indicated from the spectral analysis [32], to be dependent on the transfer rate of turbulent energy from lower wave-numbers to higher wave-numbers. The role of the fluctuation pressure can be divided into two parts: the rapid part and the slow part. This division is suggested by the solution of the Poisson equation for the fluctuating pressure field which contains two terms: one that is quadratic in the fluctuating velocity field and is responsible for the return to isotropy of an-isotropic homogeneous turbulence, the other is linear in the fluctuating velocity field and mean velocity gradient and responds immediately to applied mean strain fields.

Three assumptions are made in modeling the pressure force term and viscous force term of Eq. (3), i.e.

1. The stochastic fluctuations in the momentum of fluid elements in turbulence

fields is a Markov process.

2. For the stochastic process of high Reynolds number turbulence flows, the viscous force acting on the fluid elements is assumed in proportion to $-U_i / \tau_t$ where τ_t is the characteristic time of the turbulent flow and is assumed in proportion to κ/ε. κ and ε are the turbulent kinetic energy and its dissipation rate, respectively.

3. The local fluctuating pressure acting on a fluid element can be treated as the sum of many small pressure forces. For high Reynolds number flows, it can be expected, from a rough use of the Central Limit Theorem, that the fluctuation of momentum due to the pressure force can be simulated as a Wiener process with a Gaussian distribution.

According to Eq. (3) and assumptions 2 and 3, in an infinitesimal time interval dt, the dynamic equations for the change of momentum fluctuations of fluid elements are proposed as

$$dU_i = \left(\begin{array}{l} -U_j \dfrac{\partial < u_i >}{\partial X_j} + \dfrac{\partial < U_i U_j >}{\partial X_j} \\ \\ + A_i(t) - C_1 \dfrac{\kappa}{\varepsilon} U_i \end{array} \right) dt \quad (4)$$

where $A_i(t)$ represents a Wiener process with Gaussian distribution. From assumption 1, there exists a tpdf function Tr(t,X,V) connecting two neighboring points in the phase space. The stochastic process is completely defined by this tpdf. Let f(t,X,V) be the Eulerian pdf of the velocity fluctuations in a turbulence field. Then f(t,X,V)dV is the probability of a fluid element falling between V and V+dV in the phase space. Next, we define n(t,X,V) as the mass fraction of the chemically reactive species which are contained in and carried by the fluid elements. With the foregoing definitions of f and n, we now define the distribution function of the chemical species as

$$F(t, X, V) = n(t, X, V) f(t, X, V) \quad (5)$$

This quantity is defined such that F(t,X,V)dV denotes the mass fraction of the chemical species with velocities between V and V+dV at t and X. The probability average of n, <n> , is then

$$< n >= \int F dV \quad (6)$$

The governing equation for F is formulated herein. By setting n=1, we then readily obtain the governing equation for f. The present study will be confined to the simple chemical reactions which proceed according to the equation,

$$\left(\frac{\partial n}{\partial t}\right)_{chem} = \omega \quad (7)$$

We assume that the molecular diffusion into and out of the fluid element takes place in accordance with the value of $D\partial^2 n/\partial X_k \partial X_k$ observed in that fluid element. With the above arguments, $F(t+\Delta t, X+\Delta X, V)$ can be related to $F(t, X, V-\Delta V)$ by means of the tpdf, Tr, in the following way,

$$\begin{aligned} & F(t+\Delta t, X+\Delta X, V) = \\ & \iiint [F(t, X, V-\Delta V) + \omega f \bullet \Delta t \\ & + D\left(\frac{\partial^2 n}{\partial X_k^2}\right)_{t,X,V-\Delta V} \bullet f(t, X, V-\Delta V) \bullet \Delta t] \\ & \bullet Tr(t, X, V-\Delta V; \Delta V) d\Delta V \end{aligned} \quad (8)$$

The above equation can be transformed into a differential equation by expanding the various functions in the Taylor series small value of Δt. Once the tpdf, Tr, is found, the pdf governing the equation can be obtained. In order to evaluate the tpdf, one must solve Eq. (4) as Chung did [12].

In the present analysis, the time interval, Δt, is chosen to be much greater than the Kolmogorov's time scale, but less than the characteristic time of the large eddies. The tpdf are then constructed from the formal solution of Eq. (4) with the aid of the auxiliary lemma in previous subsection as

$$Tr(t, X, V; \Delta R) =$$

$$\left(\frac{1}{4\pi q \Delta t}\right)^{3/2}$$

$$\bullet \exp\left[-\left(\frac{\Delta R_1^2}{4q\Delta t} + \frac{\Delta R_2^2}{4q\Delta t} + \frac{\Delta R_3^2}{4q\Delta t}\right)\right] \quad (9)$$

where

$$\Delta R_i = \Delta V_i - C_i \Delta t + O\left(\Delta t^2\right)$$

$$C_i = -V_i \frac{\partial \langle u_i \rangle}{\partial X_j} + \frac{\partial \langle u_i u_j \rangle}{\partial X_j} - C_1 \frac{k}{\varepsilon} V$$

Then, after a considerable manipulation and discarding the terms of order $(\Delta t)^2$ and higher, the pdf governing equation for F was obtained as

$$\frac{\partial F}{\partial t} + u_i \frac{\partial F}{\partial X_i} =$$

$$\frac{\partial}{\partial V_i}\left[\left(V_j \frac{\partial < u_i >}{\partial X_j} - \frac{\partial < U_i U_j >}{\partial X_j} + C_1 \frac{\kappa}{\varepsilon} V_i\right) F\right]$$

$$+ \frac{\partial^2 (qF)}{\partial V_i^2} + Df \frac{\partial^2 n}{\partial X_k^2} + \omega f \quad (10)$$

where q is a undefined quantity generated from the transition moments.

Kolmogorov's hypothesis of local isotropy states [33] that if the turbulence is locally isotropic one can express the following relation by properly choosing the time scale τ,

$$\overline{\Delta U_i \Delta U_j} = C_O \varepsilon \tau \delta_{ij}$$

$$\text{for } \tau_\eta << \tau << T_O \quad (11)$$

where $\Delta U_i = U_i(t+\tau) - U_i(t)$, τ_η is the Kolmogorov's time scale, T_O is the characteristic time scale of mean turbulence fields, and C_O is a universal constant.

In deriving the tpdf, the time interval was carefully chosen to fall between the scales of small and large eddies. Therefore the time interval chosen should be of the same range as that in Kolmogorov's locally isotropic turbulence hypothesis. Then one can expect that,

$$q = C_2 \varepsilon \quad (12)$$

By substituting Eq. (12) into Eq. (10), a Fokker-Planck type pdf equation is obtained as

$$\frac{\partial F}{\partial t} + u_i \frac{\partial F}{\partial X_i} =$$

$$\frac{\partial}{\partial V_i}\left[\left(V_j \frac{\partial < u_i >}{\partial X_j} - \frac{\partial < U_i U_j >}{\partial X_j} + C_1 \frac{\kappa}{\varepsilon} V_i\right) F\right]$$

$$+ C_2 \varepsilon \frac{\partial^2 F}{\partial V_i^2} + Df \frac{\partial^2 n}{\partial X_k^2} + \omega f \quad (13)$$

Equation (13) is based on the aforementioned three assumptions which may miss some salient effects on turbulence. There several comments can be made. First, it should be seen that assumption 2 implies that the viscosity mainly plays the role of dissipating turbulent energy. However, when close to the wall, the viscosity diffusion become important. Accordingly, an additional term should be added to Eq. (13) to take care of this viscous effect more completely through the aid of Lundgren's pdf equation [20]. Second, in assumption 3, the Wiener process was proposed to simulate the effect of fluctuating pressure acting on the fluid elements. The pressure fluctuations, however, are partly affected by the mean strain rate which exhibits a strong directional character. If the mean strain rate is large, the distribution of the pressure force will become non-Gaussian. The Wiener process assumption would cause the loss of the non-Gaussian effect of the mean strain rate. Since the pressure effects were studied

extensively in Reynolds stress modeling [27,28,34-40], the lost non-Gaussian effect will be recovered by comparing Equation (13) with the pdf equation developed by Hong et al. [13]. Additionally, the pressure diffusion effect was not considered in the above modeling process. With the assistance of Lundgren's pdf equation [20] and Lumley's suggestion [39] for the pressure diffusion effect, this effect will be proposed and added to Eq. (13).

Equation (13) can be reduced to the governing equation for f by setting n=1 and ω=0 as follows.

$$\frac{\partial f}{\partial t}+u_i\frac{\partial f}{\partial X_i}= \frac{\partial}{\partial V_i}\left[\left(V_j\frac{\partial <u_i>}{\partial X_j}-\frac{\partial <U_iU_j>}{\partial X_j}\right)f + C_1\frac{\kappa}{\varepsilon}V_i\right] + C_2\varepsilon\frac{\partial^2 f}{\partial V_i^2} \quad (14)$$

The above equation with the missed terms discussed in the foregoing paragraph can be re-expressed as

$$\frac{\partial f}{\partial t}+u_i\frac{\partial f}{\partial X_i}= \frac{\partial}{\partial V_i}\left[\left(V_j\frac{\partial <u_i>}{\partial X_j}-\frac{\partial <U_iU_j>}{\partial X_j}\right)f + C_1\frac{\kappa}{\varepsilon}V_i\right] + C_2\varepsilon\frac{\partial^2 f}{\partial V_i^2}+\mathrm{D}_\nu+\mathrm{D}_\mathrm{p}+\mathrm{PS}_\mathrm{r} \quad (15)$$

where D_v, D_p and PS_r stand for the effects of viscous diffusion, pressure diffusion and the rapid part of fluctuating pressure, respectively. The Lundgren's pdf equation [31] is

$$\frac{\partial f}{\partial t}+u_i\frac{\partial f}{\partial X_i}= \frac{\partial}{\partial V_i}\left[\left(V_j\frac{\partial <u_i>}{\partial X_j}-\frac{\partial <U_iU_j>}{\partial X_j}\right)f\right] + \frac{1}{\rho}<\frac{\partial f_1}{\partial V_i}\frac{\partial P}{\partial X_i}>-<\nu\frac{\partial^2 U_i}{\partial X_j^2}\frac{\partial f_1}{\partial V_i}> \quad (16)$$

or

$$\frac{\partial f}{\partial t}+u_i\frac{\partial f}{\partial X_i}= \frac{\partial}{\partial V_i}\left[\left(V_j\frac{\partial <u_i>}{\partial X_j}-\frac{\partial <U_iU_j>}{\partial X_j}\right)f\right] + \frac{1}{\rho}<\frac{\partial^2 <f_1P>}{\partial V_i\partial X_i}>+\nu\frac{\partial^2 f}{\partial X_j^2} + \frac{1}{\rho}\frac{\partial^2 <f_1P\frac{\partial U_j}{\partial X_i}>}{\partial V_i\partial V_j} - <\nu\frac{\partial U_i}{\partial X_j}\frac{\partial U_k}{\partial X_j}\frac{\partial^2 f_1}{\partial V_i\partial V_k}> \quad (17)$$

where f_1 is the fine-grained density which is defined as

$$f_1=\delta(U(t,X)-V) = f_1(t,X;V) \quad (18)$$

and the ensemble average of the fine-grained density is the pdf f, i.e.

$$f\equiv\left\langle f_1\right\rangle \quad (19)$$

The last four terms of the RHS for Eq. (17) are obtained from the two unclosed terms in Eq. (16) which are due to the effects of the pressure and viscous forces, respectively. The first term involving derivatives of X_i and V_i indicates the pressure diffusion transport.

The second term involved a derivative with respect to V_i only denotes the pressure redistribution of f in V space. The third term is the molecular transport of f. The last term would result in viscous dissipation which can be obtained by multiplication by V_iV_j and integration over V space. The terms D_ν, D_p and PS_r appearing in Eq. (15) are obviously related to the last four terms of Eq. (17). From the previous analysis Eq. (13) keeps the effect of the last term of Eq. (17) under the condition of isotropic dissipation. In the present analysis, we let D_ν take care of the molecular viscous effect on the transport of f which is significant in the near wall region. As mentioned previously, the Wiener process maintains the slow effect of fluctuating pressure only, thus the PS_r term should contain the remaining rapid part. The PS_r will be inquired through the aid of Hong et al.'s pdf equation. Hong et al.'s pdf equation [13] is

$$\frac{\partial f}{\partial t}+u_i\frac{\partial f}{\partial X_i}= \frac{\partial}{\partial V_i}\left[\left(\begin{array}{l} V_j\dfrac{\partial <u_i>}{\partial X_j}(1-C_p)+ \\ C_{f1}\dfrac{\varepsilon}{\kappa}V_i-\dfrac{\partial <U_iU_j>}{\partial X_j}\end{array}\right)f\right] +\nu\frac{\partial^2 f}{\partial X_i^2} +\left(\begin{array}{l} C_{f2}\varepsilon- \\ \dfrac{C_p}{3}\dfrac{\partial <u_m>}{\partial X_n}<U_mU_n>\end{array}\right)\frac{\partial^2 f}{\partial V_i^2} \qquad (20)$$

From the argument by Hong et al. [13] in modeling Eq. (20), it is indicated that PS_r in Eq. (15) corresponds to the terms involved in C_p in Eq. (20).

On the other hand, when Eq. (15) is compared with (17), it also shows that D_p is equal to the second term on the RHS of Eq. (17). With regard to this pressure diffusion term appearing in the Reynolds stress equation, Lumley [39] suggested a simple relation as,

$$\frac{1}{\rho}\frac{\partial}{\partial X_i}\left\langle PU_j\right\rangle = C*\frac{\partial}{\partial X_i}\left\langle U_jU_kU_k\right\rangle \qquad (21)$$

where the constant C* takes the value –0.2. Although the validity of Eq. (21) is unclear [41,42], it is expedient to use this relation for modeling the pressure diffusion term. It is readily seen from the second term on the RHS of Eq. (17) and Eq. (21) that the simplest possible model for D_p is

$$D_p = C*\frac{\partial^2(fV_kV_k)}{\partial X_i\partial V_i} \qquad (22)$$

With the above proposed models, the transport equation for f is

$$\frac{\partial f}{\partial t}+u_i\frac{\partial f}{\partial X_i}= \frac{\partial}{\partial V_i}\left[\left(\begin{array}{l} V_j\dfrac{\partial <u_i>}{\partial X_j}(1-C_p) \\ +C_1\dfrac{\varepsilon}{\kappa}V_i-\dfrac{\partial <U_iU_j>}{\partial X_j}\end{array}\right)f\right] +\nu\frac{\partial^2 f}{\partial X_i^2} +\left(C_2\varepsilon-\frac{C_p}{3}\frac{\partial <u_m>}{\partial X_n}<U_mU_n>\right)\frac{\partial^2 f}{\partial V_i^2} +C*\frac{\partial^2(fV_kV_k)}{\partial X_i\partial V_i} \qquad (23)$$

The modeling constants C_1 and C_2 will be determined by comparison of the moment equations derived from Eq. (23) and the corresponding equation derived from the Navier-Stokes equation. The moment equation for U_kU_k derived from Eq. (23) is

$$\frac{\partial\langle U_k U_k\rangle}{\partial t}+\langle u_i\rangle\frac{\partial\langle U_k U_k\rangle}{\partial X_i}=$$
$$-\frac{\partial\langle U_i U_k U_k\rangle}{\partial X_i}-2\langle U_i U_k\rangle\frac{\partial\langle u_k\rangle}{\partial X_i}$$
$$+2(3C_2-2C_1)\varepsilon+\nu\frac{\partial^2\langle U_k U_k\rangle}{\partial X_j^2}$$
$$-2C^*\frac{\partial\langle U_i U_k U_k\rangle}{\partial X_i} \qquad (24)$$

and the turbulent energy equation derived from the Navier-Stokes equation is

$$\frac{\partial\langle U_k U_k\rangle}{\partial t}+\langle u_i\rangle\frac{\partial\langle U_k U_k\rangle}{\partial X_i}=$$
$$-\frac{\partial\langle U_i U_k U_k\rangle}{\partial X_i}-2\langle U_i U_k\rangle\frac{\partial\langle u_k\rangle}{\partial X_i}$$
$$-2\nu\left\langle\frac{\partial U_k}{\partial X_j}\frac{\partial U_k}{\partial X_j}\right\rangle+\nu\frac{\partial^2\langle U_k U_k\rangle}{\partial X_j^2}$$
$$-2\frac{\partial\langle PU_k/\rho\rangle}{\partial X_k} \qquad (25)$$

When Eq. (24) is compared with Eq. (25) and using Eq. (21), one can obtain the relationship between C_1 and C_2.

$$C_2=\frac{(2C_1-1)}{3} \qquad (26)$$

The $\langle U_iU_j\rangle$ moment equation derived from Eq. (23) is

$$\frac{\partial\langle U_i U_j\rangle}{\partial t}+\langle u_k\rangle\frac{\partial\langle U_i U_j\rangle}{\partial X_k}=$$
$$-\frac{\partial\langle U_i U_j U_k\rangle}{\partial X_k}-\langle U_j U_k\rangle\frac{\partial\langle u_i\rangle}{\partial X_k}$$
$$-\langle U_i U_k\rangle\frac{\partial\langle u_j\rangle}{\partial X_k}-\frac{2}{3}\varepsilon\delta_{ij}+\nu\frac{\partial^2\langle U_i U_j\rangle}{\partial X_k^2}$$
$$-2C_1\frac{\varepsilon}{\kappa}\left[\langle U_i U_j\rangle-\frac{1}{3}\delta_{ij}\langle U_k U_k\rangle\right]$$
$$-C^*\frac{\partial}{\partial X_n}\begin{bmatrix}\langle U_m U_m U_i\rangle\delta_{jn}\\+\langle U_m U_m U_j\rangle\delta_{in}\end{bmatrix}$$
$$+C_p\begin{bmatrix}\langle U_j U_k\rangle\dfrac{\partial\langle u_i\rangle}{\partial X_k}+\langle U_i U_k\rangle\dfrac{\partial\langle u_j\rangle}{\partial X_k}\\-\dfrac{2}{3}\delta_{ij}\langle U_m U_n\rangle\dfrac{\partial\langle u_m\rangle}{\partial X_n}\end{bmatrix} \qquad (27)$$

When we compare Eq. (27) with the corresponding equations derived from the Navier-Stokes equation [43], it shows that the two are identical if

$$-2C_1\frac{\varepsilon}{\kappa}\left[\langle U_i U_j\rangle-\frac{1}{3}\delta_{ij}\langle U_k U_k\rangle\right]$$
$$-C^*\frac{\partial}{\partial X_n}\begin{bmatrix}\langle U_m U_m U_i\rangle\delta_{jn}\\+\langle U_m U_m U_j\rangle\delta_{in}\end{bmatrix}$$
$$+C_p\begin{bmatrix}\langle U_j U_k\rangle\dfrac{\partial\langle u_i\rangle}{\partial X_k}+\langle U_i U_k\rangle\dfrac{\partial\langle u_j\rangle}{\partial X_k}\\-\dfrac{2}{3}\delta_{ij}\langle U_m U_n\rangle\dfrac{\partial\langle u_m\rangle}{\partial X_n}\end{bmatrix}$$
$$-\frac{2}{3}\varepsilon\delta_{ij}=\frac{1}{\rho}\left\langle P\left(\frac{\partial U_j}{\partial X_i}+\frac{\partial U_i}{\partial X_j}\right)\right\rangle$$
$$-\frac{1}{\rho}\left(\frac{\partial\langle PU_j\rangle}{\partial X_i}+\frac{\partial\langle PU_i\rangle}{\partial X_j}\right)$$
$$-2\nu\left\langle\frac{\partial U_i\partial U_j}{\partial X_m\partial X_m}\right\rangle \qquad (28)$$

The last term on the RHS represents the viscous dissipation which is rationally presumed to be isotropic at a high Reynolds number. Hence this term is identical to the third term on the LHS. The second term on the RHS is
the pressure diffusion, which can be equal to the last term on the LHS if Lumley's suggestion for D_p shown in Eq. (21) is accepted. The remaining terms in Eq. (28) are

$$C_p\left[\begin{array}{l}\left\langle U_j U_k\right\rangle\frac{\partial\left\langle u_i\right\rangle}{\partial X_k}+\left\langle U_i U_k\right\rangle\frac{\partial\left\langle u_j\right\rangle}{\partial X_k}\\ -\frac{2}{3}\delta_{ij}\left\langle U_m U_n\right\rangle\frac{\partial\left\langle u_m\right\rangle}{\partial X_n}\end{array}\right]$$
$$-2C_1\frac{\varepsilon}{\kappa}\left[\left\langle U_i U_j\right\rangle-\frac{1}{3}\delta_{ij}\left\langle U_k U_k\right\rangle\right]$$
$$=\frac{1}{\rho}\left\langle P\left(\frac{\partial U_j}{\partial X_i}+\frac{\partial U_i}{\partial X_j}\right)\right\rangle \qquad (29)$$

Equation (29) is identical to the relationship between the stress and the pressure-strain (P-S) cor-relations derived by Rotta [34] and Naot et al. [35], respectively, for modeling the slow and rapid parts of P-S cor-relations. Therefore, Eq. (27) is term-wise comparable with the proved Reynolds stress model except for the third order correlation terms. In the Reynolds-stress closure, a model for the third order cor-relations is required but, in the pdf equation, the corresponding term appears in closed form. Hence the pdf model can be expected to be reliable since it is compatible with proven Reynolds-stress closures.

Corresponding to the proven Reynolds-stress closures, the modeling constants C_1 and C_p can be determined. Following Launder argument [44], the choices of C_1 and C_p fit approximately the relationship

$$\frac{(1-C_p)}{C_1}=0.46 \qquad (30)$$

Therefore, for various turbulent flows the constants C_1 and C_p, and then C_2 by virtue of Eq. (26), can be adopted to capture a much better flow structure. For more on this variation of choosing C_1 and C_p, please refer to Launder's paper [44].

A similar comparison can be made between the moment equation derived from the pdf equation including the variable n and the classically derived moment equations for the chemical species n. First, the pdf equation including n corresponding to Eq. (23) must be obtained. Equation (23) can be readily generalized to construct the governing equation of chemical species when following Chung's work [45]. The resulting pdf equation is

$$\frac{\partial F}{\partial t}+u_i\frac{\partial F}{\partial X_i}=$$
$$\frac{\partial}{\partial V_i}\left[\left(\begin{array}{l}V_j\frac{\partial<u_i>}{\partial X_j}(1-C_p)\\ +C_1\frac{\varepsilon}{\kappa}V_i-\frac{\partial<U_iU_j>}{\partial X_j}\end{array}\right)F\right]$$
$$+\nu\frac{\partial^2 F}{\partial X_i^2}$$
$$+\left(\begin{array}{l}C_2\varepsilon-\\ \frac{C_p}{3}\frac{\partial<u_m>}{\partial X_n}<U_mU_n>\end{array}\right)\frac{\partial^2 F}{\partial V_i^2}$$
$$+C^*\frac{\partial^2(FV_kV_k)}{\partial X_i\partial V_i}+Df\frac{\partial^2 n}{\partial X_k^2}+\omega f \qquad (31)$$

The moment equation for the chemical species can be derived by taking the moment of Eq. (31) with respect to U_i. The resulting equation is

$$\frac{\partial\left\langle n\right\rangle}{\partial t}+\frac{\partial\left\langle u_i n\right\rangle}{\partial X_i}=(\nu+D)\frac{\partial^2\left\langle n\right\rangle}{\partial X_i^2}+\left\langle\omega\right\rangle \qquad (32)$$

which is the same as the standard species conservation equation. It is interesting to note that for the conservation equations of <n > derived from Eq. (31), the terms involving derivatives of V_i make no contribution: their

effect is on the second moments.

We have now shown that the moment equations for velocity cor-relations and n derived, respectively, from Eqs. (23) and (31) are equivalent to the corresponding equations derived from the Navier-Stokes equation and the standard species conservation equation. Therefore, solutions for Eqs. (23) and (31) give a complete description of the non-isotropic turbulent reactive flow field, at least to the extent that it satisfies these fundamental moment equations.

4.Self-review

A pdf model equation has been constructed which describes the statistical behavior of fluid elements containing chemically reactive species. This pdf equation has been derived and adapted to govern the pdf of the fluid elements and, hence, of the chemical species. It is noted that the present model differs from that of treating the pdf for the chemical species, in which the species mass fraction is itself an independent variable. The dependent variable F appearing in Eq. (31) is defined such that the ensemble average of the species mass fraction is as shown in Eq. (6). As it is implicit in Eq. (6), the probability of finding a scalar quantity is closely related to that of finding a fluid element containing the scalar quantity, therefore, the distribution function of the scalar quantity is expressed in terms of the fluid element as

$$P(t, X, n) \rightarrow F(t, X, V)dV \qquad (33)$$

Note that, without the above relationship, one must generate pdf equations for distribution functions of all possible combination of n's and u's, which would render the analysis intractable. The above fact enables us to limit the independent variables to t, X, and V, for both the pdf of fluid elements and the chemical species. This is a critical aspect of the present model in rendering the model tractable with little sacrifice in accuracy. The present model makes it possible to explore the behaviors of turbulent reactive flows by virtue of the velocity space dependence.

Subsequently, we will make a comparison of the fundamental aspects of the present pdf model with Chung's [12] and Pope's [5] models. We will briefly discuss the major differences among these models. Their differences can be seen clearly from the starting point and the final form of each model. The starting point of the present model and Pope's model is the Navier-Stokes equation, whereas Chung's model is a thoroughly different one. Chung assumed that the statistical property of a fluid element is entirely due to the lower non-equilibrium wave-number, and that the role of higher equilibrium wave-number is to degenerate to a random state and dissipate this property by their interaction with lower wave-numbers. When the Reynolds number is sufficiently large, a statistical separation exists between the higher and lower wave-numbers across an inertial sub-range. The dynamics of various wave-numbers in turbulence fields could be seen as closely related to Prigogine's description of generalized Brownian motion. Thus Chung employed Langevin's stochastic equation of the generalized Brownian motion to describe the momentum change of a fluid element under the interaction of large and small size eddies at high Reynolds number flow.

Concerning the final forms, term by term can be compared between the present model and Pope's and Chung's models except for two major differences. The first discrepancy is that the present and Chung models are in a tractable manner without the terms involving the derivative and the integral with respective to the chemical species which appears in the Pope model. The second discrepancy is that the highest derivative order with respective to physical space in the present model is two and in the Pope's and Chung's models it is one. The second order derivative term, although being negligible in most regions of the flow field, becomes important near a solid wall region and keeps the elliptic characteristic of the pdf equation. The moment equations were derived from the present model, and they were shown to be identical up to the term, to those derived from the Navier-Stokes equation, thus

establishing the basic consistency of the present model. The relationship between the model constants appearing in the present pdf equation have been constructed, which would render the present model completely self-containing for chemically reactive flows. Future research efforts would aim at solving this pdf equation for appropriate turbulent flows for the sake of validating this new model.

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