Inverse parabolicity of PDF equations in turbulent flows – reversed-time diffusion or something else

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1. Motivation

The focus of the present work is the well-known feature of the PDF transport equations in turbulent flows – the inverse parabolicity of the equations. While it is quite common in fluid mechanics to interpret equations with direct (forward-time) parabolicity as either diffusion or a combination of diffusion and other processes (for example convection and reaction), the possibility of a similar interpretation for the equations with inverse parabolicity is not clear. In the present work, we investigate whether the inverse-parabolic terms in PDF equations can be treated as an "inverse diffusion". In other words, we look for a physical process which can be modeled by this inverse diffusion while complying with the major laws of nature and turbulence.

2. The PDF transport equations

The PDF techniques, which have been developed for last thirty years, represent an effective tool for deriving and analyzing the PDF transport equations in turbulent flows (Pope 1985, Kuznetsov & Sabelnikov 1989, Dopazo 1894, Klimenko & Bilger 1999, Pope 2000). The PDF transport equation

$$\frac{\partial P}{\partial t}+\frac{\partial \hat{u}_i P}{\partial x_i}+\frac{\partial \hat{A}_I P}{\partial z_I}+\frac{\partial^2 \hat{B}_{IJ} P}{\partial z_I \partial z_J}=0 \tag{2.1}$$

specifies the evolution of a joint PDF $P = P(\mathbf{z}; \mathbf{x}, t)$ of the values $\mathbf{Z} = (Z_1, ..., Z_n)$ which are transported by the turbulence according to

$$\frac{\partial Z_I}{\partial t}+\frac{\partial v_i Z_I}{\partial x_i}-D\frac{\partial^2 Z_I}{\partial x_i \partial x_i}=W_I \tag{2.2}$$

Here we introduce the conditional expectation $\hat{u}_i(\mathbf{z}, \mathbf{x}, t)$ of velocity $v_i(\mathbf{x}, t)$, the conditional dissipation $\hat{B}_{IJ}(\mathbf{z}, \mathbf{x}, t)$, which is, by definition, symmetric and positive semidefinite and the conditional "drift" coefficient $\hat{A}_I(\mathbf{z}, \mathbf{x}, t)$ according to the following equations

$$\hat{u}_i \equiv \langle v_i|\mathbf{Z}=\mathbf{z}\rangle\,,\quad \hat{B}_{IJ} \equiv \langle D\boldsymbol{\nabla} Z_I\cdot\boldsymbol{\nabla} Z_J|\mathbf{Z}=\mathbf{z}\rangle\,,\quad \hat{A}_I \equiv \langle W_I|\mathbf{Z}=\mathbf{z}\rangle \tag{2.3}$$

By default, the lower case indices run over physical coordinates (that is $i = 1, 2, 3$) while the upper case indices run over all dimensions of the transported quantities (that is $I = 1, 2, 3, 4, ..., n$). Vector notation is used to denote vectors of maximal dimension introduced for a particular quantity. For example, $\mathbf{x} = (x_1, x_2, x_3) = (x_i; i = 1, 2, 3)$ and $\mathbf{Z} = (Z_1, ..., Z_n) = (Z_I; I = 1, ..., n)$. The sample space variable for $\mathbf{Z}$ is denoted by $\mathbf{z}$. The convention of summation over repeated indices applies throughout the paper. The gradient operators are calculated in the physical space $\boldsymbol{\nabla} = (\partial/\partial x_i,\ i = 1, 2, 3)$ For simplicity,

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we assume that the density ρ is constant, and that the Reynolds number is high so that the terms involving transport by molecular diffusion (such as those specified by the term $D\nabla^2 P$) and differential-diffusion effects can be neglected. Apart from these conventional assumptions, equation (2.1) is exact and can be derived from (2.2) by standard PDF techniques (Pope 1985, Kuznetsov & Sabelnikov 1989, Dopazo 1894, Klimenko & Bilger 1999 and Pope 2000). The physical meaning of the values W_I depends on the actual physical meaning of the variables Z_I: for reactive scalars W_I would represent a chemical source term while for velocity components W_I denotes the pressure gradient. For the sake of certainty, we assume that the first three components of Z_I represent the velocity components, while the rest of the values Z_I (that is Z_4, ..., Z_n) are reactive scalars. Thus we have

$$v_i = Z_i,\ \hat{u}_i = z_i,\ W_i = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} \tag{2.4}$$

while the other source terms $W_\alpha = (W_4, ..., W_n)$ are assumed to be functions of the scalar variables $W_\alpha = W_\alpha(Z_4,\ ...,\ Z_n)$ and their particular forms are not stipulated in the present work. By default, the Greek indices run over the "scalar quantities" $\alpha = 4, ..., n$.

The most interesting feature of (2.1) is its inverse parabolicity, determined by the positive sign of the last term. While direct parabolic equations are quite common in fluid mechanics and other areas of engineering, inverse-parabolic equations seem quite unusual for any physical process but they are most common for the PDF equations in turbulent flows. The objective of the present work is to find a reasonable physical interpretation of this strange but common feature of the PDF equations.

3. The reversed-time diffusion model

The terms with conventional direct parabolicity, such as the last term on the left-hand side of (2.2), are called the diffusion terms, since these terms may normally be associated with some diffusive Markov processes (or random-walk processes). For example, the diffusion of a small amount of dye in stationary fluid is governed by (2.2) with $\mathbf{v} = 0$ and $W = 0$. In this case the word "diffusion" reflects existence of the physical molecular diffusion process represented by a random walk of the dye molecules causing spreading of the dye into uncolored fluid. The Markov diffusion process specified by the Ito stochastic equation $dx_i^* = (2D)^{1/2} dw_i^*$ would represent a good mathematical model of this molecular random-walk provided the value D matches the physical value of the diffusion coefficient (here w_i^* represent independent Wiener processes which are commonly used in constructing stochastic models). We should note that the Markov diffusion process is not necessarily identical to the physical random-walk of the dye molecules but the former would certainly represent an adequate mathematical model of the latter. Thus the physical interpretation of the equations involving direct parabolicity is, usually, not very difficult: using the Ito equations, one can build a Markov diffusion process which corresponds to the original diffusion equation. This Markov process should represent a reasonable model of the physical process which is described by the diffusion equation, provided that the coefficients of the Ito equation are matched well with the corresponding physical properties.

On the face of the problem the physical interpretation of the inverse-parabolic equation (2.1) is only marginally more complicated than the problems considered in the previous paragraph. One needs to introduce the reversed time $\tau \equiv -t$ and rewrite (2.1) as an equation with direct parabolicity,

$$\frac{\partial F^-}{\partial \tau}+\frac{\partial u_i^- F^-}{\partial x_i}+\frac{\partial A_I^- F^-}{\partial z_I}-\frac{\partial^2 \hat{B}_{IJ} F^-}{\partial z_I \partial z_J}=0 \tag{3.1}$$

where

$$A_I^- \equiv -A_I,\ \ u_i^- \equiv -\hat{u}_i,\ \ \tau \equiv -t.$$

Equation (3.1), obviously, satisfied by $F^- = P$ and, at the same time, it can be interpreted as the reversed-time Fokker-Planck equation (with drift coefficients u_i^- and A_I^- and the diffusion coefficients $\hat{B}_{IJ}$) which governs the transitional probabilities for the Ito equation represented by the following system of stochastic equations

$$dx_i^- = u_i^- d\tau,\ dz_I^- = A_I^- d\tau + b_{IJ} \overset{\text{Ito}^-}{\cdot}\ dw_J^- \tag{3.2}$$

where $\hat{B}_{IJ} = b_{IK} b_{JK}/2$ and w_J^- represents the Wiener processes driving the stochastic processes z_I^- and x_i^- backward in time. The symbol "Ito$^-$" indicates that the product should be evaluated in the "Ito sense" backward in time, that is, if $d\tau$ is positive, b_{IJ} is evaluated at τ but not at $\tau + d\tau$. This interpretation of the PDF equation is formally correct – the PDF of the constructed Markov process should coincide with P (provided the values of the coefficients $\hat{u}_i,\ \hat{A}_I$ and $\hat{B}_{IJ}$ are specified in agreement with their physical definitions (2.3) and the initial distribution for the stochastic trajectories are set in accordance with P). We use a new function F^- in (2.1), since in addition to $F^- = P$, the function F^- may represent other solutions of the Fokker-Planck equation, depending also on normalization and the initial conditions (for example, the transitional probabilities).

Although the constructed stochastic process models the PDF P well, we must refrain from claiming any deeper similarity between the model and some physical processes in turbulent flows (as we did while considering molecular diffusion of dye controlled by equations with direct parabolicity). It is not obvious if (and how) the stochastic trajectories specified by (3.2) can be associated with some physical trajectories. Indeed, all physical processes evolve forward in time while the constructed model develops backward in time, and it would be very difficult to specify a physical process which can correspond to the model. In order to illustrate this difficulty we introduce the following notation:

- *Realization of the process* – a particular trajectory represented by a specific solution of the Ito equation;
- *Markov process* – combines many realizations according to their probabilities. The Markov process is characterized by the diffusion and drift coefficients and by a certain PDF (such as P) which satisfies the Fokker-Planck equation and certain initial conditions;
- *Markov family* – is characterized by certain diffusion and drift coefficients but comprise many Markov processes which correspond to different solutions of the same Fokker-Planck equation with different initial conditions. The family does not correspond to a single PDF (such as P) but to all possible PDFs satisfying a given Fokker-Planck equation.

In the case of dye diffusion, we found that not only a particular Markov process, but also its family, correspond well to the physics of the problem (indeed, let us consider diffusion of the dye as a passive substance with different initial conditions). In the case of the reversed-time process, only the modeling Markov process is assigned a certain physical significance, not its family. This can be illustrated by the following consideration. Let us assume that at $t = t_0$ (and $\tau = \tau_0 \equiv -t_0$) the PDF is slightly altered due to some external influence $F^- = P + F'$ instead of $F^- = P$. Physically, the F^- would be different from its original prognosis P for some time after t_0 (that is for $t > t_0$) while the PDF F^- of the process specified by (3.1) and (3.2) would differ for some time before t_0 (that is $\tau > \tau_0$). This illustrates that the coefficients of (3.1) and (3.2) must change for $t > t_0$ if the PDF is disturbed at $t = t_0$. Hence, although the Markov process $F^- = P$ models the actual joint PDF P, the other processes from the same Markov family (represented by the other solutions of the same equation (3.1)) do not correspond well to the physical processes in turbulent flows.

4. The forward-time diffusion model

The difficulties that we experienced in the previous section in finding a good physical interpretation of the reversed-time diffusion model are, obviously, related to the fact that physical processes develop forward in time. Thus, it would be desirable to reverse the reversed-time process and force it to develop forward in time. We have a Markov process with the PDF $F^- = P$ which evolves backward in time, and we wish to find another Markov process which evolves forward in time and which is equivalent to the original process. That is, if the trajectories of the first process are shown on a photograph, they are indistinguishable from the trajectories of the second process. However, one can easily distinguish the processes while watching their animated evolutions – they will propagate in opposite directions. The possibility of reversing a Markov process is not obvious, but is proved in the special Anderson (1982) theorem. It should also be noted that only a specific Markov process, but not its whole Markov family, can be reversed in time, and the original and reversed processes may belong to different Markov families. The original and reversed processes form adjoint couples – an attempt to reverse the reversed process once more yields the original process. It should be noted that, although the Fokker-Planck equation is essentially the same as the direct Kolmogorov equation of a Markov process, the inverse Kolmogorov equation of the same process should not be confused with the Fokker-Planck equation of the reversed-time process. The inverse Kolmogorov equation deals with transitional probabilities of the process, which are not specifically considered in this section.

The Anderson (1982) equations, applied to the reversed-time diffusion model specified by $F^- = P$ and by (3.1) – (3.2), indicate that the Fokker-Planck equation for the forward-time diffusion model is given by

$$\frac{\partial F^+}{\partial t} + \frac{\partial u_i^+ F^+}{\partial x_i} + \frac{\partial A_I^+ F^+}{\partial z_I} - \frac{\partial^2 \hat{B}_{IJ} F^+}{\partial z_I \partial z_J} = 0 \tag{4.1}$$

where

$$A_I^+ \equiv \hat{A}_I + \frac{2}{P}\frac{\partial \hat{B}_{IJ} P}{\partial z_J}, \quad u_i^+ \equiv \hat{u}_i$$

The Ito equation, which corresponds to (4.1), is specified by

$$dx_i^+ = u_i^+ dt, \; dz_I^+ = A_I^+ dt + b_{IJ} \overset{\text{Ito}^+}{\cdot} dw_J^+ \tag{4.2}$$

The symbol "Ito$^+$" indicates that the product should be evaluated as an Ito product forward in time, and $\hat{B}_{IJ} = b_{IK} b_{JK}/2$. The Anderson theorem provides even the possibility to reverse particular realizations of a Markov process, that is $x_i^+(-\tau) = x_i^-(\tau)$ and $z_i^+(-\tau) = z_i^-(\tau)$ provided the forward and backward Wiener processes are linked by the equation

$$dw_J^+ = dw_J^- + \Phi_A\left(\mathbf{z}^-(\tau), \mathbf{x}^-(\tau), \tau\right) d\tau, \quad \Phi_A(\mathbf{z}, \mathbf{x}, -t) \equiv \frac{1}{P}\frac{\partial b_{IJ}P}{\partial z_I} \tag{4.3}$$

We emphasize that, of course, all differentials in this equation (and in other equations of the present work) are evaluated in the same direction in time. The proof that the stochastic process w_J^+ defined by (4.3) may be treated as a Wiener process is far from trivial and can be found in Anderson (1982).

The trajectories specified by s (3.2) and (4.2) can be conventionally called "the stochastic particles". Although the stochastic trajectories specified by (4.2) coincide with the stochastic trajectories of the reversed-time model, the process (4.2) is more convenient for our purposes, since it evolves forward in time. In the following sections, we demonstrate that, for the Markov family specified by (4.2) and (4.2), its physical analog (i.e. a physical process in a turbulent flow which can reasonably be modelled by the family) can be found. The family of stochastic trajectories, which are specified by (4.2),.can be associated with some physical trajectories in a turbulent flow.

5. The physical process

We consider the Lagrangian fluid particles transported by a turbulent flow jointly with the fields specified by (2.2), and introduce the following conditional expectation:

$$Q = Q(\mathbf{z}, \mathbf{x}, t) \equiv \langle f | \mathbf{Z} = \mathbf{z} \rangle \tag{5.1}$$

where $f = f(\mathbf{x}, t)$ represents the concentration of the fluid particles. The fluid particles are transported according to the equations

$$dx_i^* = v_i(\mathbf{x}^*(t), t)dt, \qquad \frac{\partial f}{\partial t} + \frac{\partial v_i f}{\partial x_i} = 0 \tag{5.2}$$

The second equation in (5.2), representing the transport equation for f, is equivalent to the first equation in (5.2) specifying the fluid particle trajectories $\mathbf{x}^*(t)$. The function f also allows us to select some of the fluid particles (f set to 1 for the selected fluid particles and f set to 0 for others) or assign each fluid particle a certain weight f.

At this point we declare that the stochastic particles of the forward-time diffusion model are considered to be a model for the turbulent transport of fluid particles. In order to be accurate in this declaration, we should state how the properties of the particle transport are simulated by the model. Specifically, we assume that $F^+ = QP$, that is, F^+ is a model for QP. The different Markov processes which belong to the family of (4.1) are interpreted as variations of Q, while P remains the same for the whole family. Since $f = 1$ obviously satisfies (5.2) and $F^+ = P$ satisfies (4.1), the forward-time model is trivial if it is restricted only to $F^+ = P$. The assumed similarity of turbulent transport of fluid particles and a forward-time process is a hypothesis which is expected to be valid for any reasonable initial $Q \neq 1$. .

The physical interpretation of modeling stochastic trajectories needs some clarification. Let us assume that the PDF $P = P(\mathbf{z}, \mathbf{x}, t)$ is represented by a very large number of trajectories of the stochastic particles on the time interval $t_1 \leq t \leq t_2$. These trajectories can be obtained equivalently by a) solving (3.2) backward in time from the initial distribution of the particles in $\mathbf{z}$-$\mathbf{x}$-space at $t = t_2$ specified by $P(\mathbf{z}; \mathbf{x}, t_2)$; or b) solving s (4.2) forward in time from the initial distribution of the particles in $\mathbf{z}$-$\mathbf{x}$-space at $t = t_1$ specified by $P(\mathbf{z}; \mathbf{x}, t_1)$. We wish to select some of the stochastic particles so that their distribution $F(\mathbf{z}, \mathbf{x}, t)$ models the distribution of marked fluid particles in $\mathbf{z}$-$\mathbf{x}$-space for $t_1 \leq t \leq t_2$ (i.e. $F = QP$ but $Q \neq 1$ since f is different for marked and non-marked fluid particles). In order to find $F(\mathbf{z}, \mathbf{x}, t)$, we can select the stochastic particles so that their distribution at $t = t_1$ is given by $F(\mathbf{z}, \mathbf{x}, t_1)$. The particles must be selected solely on the basis of their positions in $\mathbf{z}$-$\mathbf{x}$-space at $t = t_1$ (i.e. by ignoring their future trajectories). The distribution of the selected stochastic particles for $t_1 \leq t \leq t_2$ corresponds to $F(\mathbf{z}, \mathbf{x}, t)$. (The same effect can be achieved by assigning the initial weights of $Q(\mathbf{z}, \mathbf{x}, t_1)$ to all stochastic particles. Here, $\mathbf{z}$ and $\mathbf{x}$ are determined by the location of each stochastic particle at $t = t_1$.) It should be noted that selecting the stochastic trajectories on the basis of particle positions at $t = t_2$ and the distribution $F(\mathbf{z}, \mathbf{x}, t_2)$ would not, generally, give the expected distribution $F(\mathbf{z}, \mathbf{x}, t)$ for the time interval $t_1 \leq t < t_2$. The suggested interpretation allows us to model stochastic behavior of a single fluid particle with a given initial location $\mathbf{z}_1$,$\mathbf{x}_1$ in $\mathbf{z}$-$\mathbf{x}$-space. This can be done by selecting $Q \sim \delta(\mathbf{z} - \mathbf{z}_1)\delta(\mathbf{x} - \mathbf{x}_1)$, where the Delta function applied to the vector arguments denotes the product of the Delta functions applied to the components.

In the next section, we assess the pluses and minuses of the forward-time diffusion model and its physical interpretation. This can be done by introducing a model which belongs to the same class as the forward-time diffusion model and, to the best of our knowledge, is the optimal model from this class.

6. The optimal diffusion model

Assuming that the evolution of the function $F^+ = QP$ can be specified by the following equation

$$\frac{\partial F^+}{\partial t} + \frac{\partial u_i F^+}{\partial x_i} + \frac{\partial A_I F^+}{\partial z_I} - \frac{\partial^2 B_{IJ} F^+}{\partial z_I \partial z_J} = 0 \tag{6.1}$$

with the coefficients $u_i(\mathbf{z}, \mathbf{x}, t)$, $A_I(\mathbf{z}, \mathbf{x}, t)$ and $B_{IJ}(\mathbf{z}, \mathbf{x}, t)$ which are not known a priori, the goal of this section is to find the definitions of these coefficients which comply with known properties of turbulence. The coefficients are then to be compared with the corresponding coefficients of the forward-time diffusion model. First, we note that integration of (6.1) over all z_I should result in the averaged scalar-transport equation, $\partial \langle f \rangle / \partial t + \operatorname{div} \langle \mathbf{v} f \rangle = 0$. This condition implies that

$$\int u_i Q P d\mathbf{z} = \int \hat{u}_i Q P d\mathbf{z}.$$

Since these integrals must be the same for any Q we conclude that

$$u_i = \hat{u}_i. \tag{6.2}$$

The second constraint is that $F^+ = P$ (i.e. $Q = 1$) is a solution of (6.1). This condition can be satisfied if

$$A_I = \hat{A}_I + \frac{1}{P} \frac{\partial (\hat{B}_{IJ} + B_{IJ}) P}{\partial z_J} \tag{6.3}$$

Here we use the fact that P is governed by (2.1). The third constraint is related to the Kolmogorov (1941) theory of small-scale turbulence and the Richardson (1926) law of turbulent dispersion. According to the Kolmogorov theory, the turbulent dispersion of particles at small scales (although exceeding the viscous scales of turbulence) is determined by the average dissipation of energy and, if any scalar fields are involved, by the average scalar dissipation. Since the characteristics considered here are conditional, we assume that the conditional dissipation terms $\hat{B}_{IJ}$ are to be used. The evolution of F^+ with sharp initial conditions (e.g. $F^+ \sim \delta(\mathbf{z}-\mathbf{z}_1)\delta(\mathbf{x}-\mathbf{x}_1)$ as previously considered) is determined by the diffusion term of (6.1) which is characterized by the coefficient B_{IJ}. Thus we can write

$$\mathbf{B} \sim \hat{\mathbf{B}} \tag{6.4}$$

The vector-type notation used in this equation indicates a certain link or a general compatibility of magnitudes between the values B_{IJ} and $\hat{B}_{IJ}$ and it does not mean that B_{IJ} and $\hat{B}_{IJ}$ are the same.

In order to investigate the other constraints which can be applied to the coefficients, it is convenient to rewrite (6.1) as an equation for Q

$$\frac{\partial Q}{\partial t} + \hat{u}_i \frac{\partial Q}{\partial x_i} + A_I^\circ \frac{\partial Q}{\partial z_I} - B_{IJ} \frac{\partial^2 Q}{\partial z_I \partial z_J} = S \tag{6.5}$$

where $S \equiv 0$,

$$A_I^\circ \equiv A_I - \frac{2}{P}\frac{\partial B_{IJ} P}{\partial z_J} = \hat{A}_I + \frac{1}{P}\frac{\partial(\hat{B}_{IJ} - B_{IJ})P}{\partial z_J} \tag{6.6}$$

and we take into account s (2.1), (6.2) and (6.3). Equation (6.5) corresponds to Conditional Moment Closure (CMC — Klimenko & Bilger 1999) with multiple velocity-scalar conditioning. Another constraint, which can be called "the linear constraint", is conventional in CMC and explores similarity between scalars f and $Z_4, ..., Z_n$. Indeed, since we neglect all differential diffusion effects, the conditional characteristics of the scalar f, which satisfies the equation

$$\frac{\partial f}{\partial t} + \frac{\partial v_i f}{\partial x_i} - D\frac{\partial^2 f}{\partial x_i \partial x_i} = S \tag{6.7}$$

should be similar to these of the scalar f, which satisfies (5.2). Effectively, the replacement of (5.2) by (6.7) introduces the diffusing particles of Dreeben & Pope (1997), transported by the turbulence according to

$$dx_i^* = v_i(\mathbf{x}^*(t), t)dt + \sqrt{2D}dw_i^* \tag{6.8}$$

The Brownian-type fluctuations, which are induced by the Wiener processes w_i^*, simulate the molecular-diffusion effects. In addition, if $S = S(Z_4, ..., Z_n) \neq 0$, the particles are allowed to appear (for $S > 0$) or disappear (for $S < 0$). The extension of the forward-time Markov model to these particles is reasonable since, if the Lagrangian trajectories in the phase space of the scalars $Z_4, ..., Z_n$ are well-represented by the Markov process $z_4^+(t), ..., z_n^+(t)$, then any deterministic function $S = S(z_4^+, ..., z_n^+)$ should also possess the Markov property. (Here we assume that, as in the chemical reactions, the source term S and the other source terms W_α are deterministic functions of the scalars $Z_4, ..., Z_n$). The purpose of the extension is to utilize the similarity of turbulent transport of scalars f and $Z_4, ..., Z_n$ by making the transport equation for f similar to (2.2). At this point we note that $f = a_\alpha Z_\alpha + a_0$, $S = a_\alpha W_\alpha$ form a solution of (6.7) where a_α and a_0 are arbitrary constants. Hence $Q = a_\alpha Z_\alpha + a_0$, $S = a_\alpha W_\alpha$ must satisfy (5.1). This constraint leads us to the relation $A_\alpha^\circ = \hat{A}_\alpha$ which, if we take into consideration (6.6), means in practice that

$$B_{\alpha I} = \hat{B}_{\alpha I} \tag{6.9}$$

Note that the matrices B_{JI} and $\hat{B}_{JI}$ are symmetric.

Although application of the linear constraint to the scalar quantities is a common practice in Conditional Methods, a similar constraint should not be applied to the velocity components z_i $(i = 1, 2, 3)$ (Klimenko 1998, Weinman & Klimenko 2000). Due to the specific nature of the pressure gradient, which cannot be expressed as a deterministic function of velocities and scalars, the turbulent transport of momentum is quite different from the turbulent transport of scalars. This point can be illustrated by assuming, in the spirit of (6.4), that

$$B_{ij} = \frac{3}{2} C_0 \hat{B}_{ij} \tag{6.10}$$

where C_0 is, effectively, the so-called Kolmogorov constant. The linear constraint applied to velocities would require $C_0 = 2/3$. Although this value was suggested in one of the early works (Krasnoff & Peskin 1971), the value of $C_0 = 2/3$ is not consistent with DNS and experiments for particle diffusion in turbulent flows. DNS indicate that C_0 is about 2 (Yeung & Pope 1989, Weinman & Klimenko 2000) while it is expected that $C_0 \sim 7$ when the Reynolds number becomes very large (Sawford 1991). These acceptable values for C_0 are noticeably larger than 2/3.

Comparison of the optimal diffusion model with the forward-time model indicates that all coefficients are the same with exception of B_{ij} – the 3×3 matrix of the diffusion rate in the velocity phase space. The forward-time diffusion model corresponds to $C_0 = 2/3$ which significantly underestimates the diffusion rate in the velocity space.

7. Conclusions

The transport equations for joint velocity/scalar PDFs are considered and the possibility of interpreting the inverse-parabolic terms in these equations as reversed-time diffusion has been investigated. This interpretation presumes that the reversed-time diffusion process (that is, a Markov diffusion process which corresponds to the PDF equation) can be interpreted as a model for certain physical processes in turbulence. Although we found that the physical process of Lagrangian dispersion of fluid particles in a turbulent flow may be modeled by the trajectories of the diffusion process mentioned above, this possibility needs certain qualifications:

1) Since the trajectories of the reversed-time diffusion process are propagating backwards in time, they have to be reversed in time to match the properties of fluid particles which, obviously, develop forward in time. We call the result of reversing the reversed-time diffusion process the "forward-time diffusion model".

2) The forward-time diffusion model also represents a Markov process, although it belongs to a different Markov family (i.e. the transport coefficients of the model and the original PDF equation are not the same). The forward-time diffusion process is naturally associated with the original PDF transport equation and, at the same time, has a direct link to the equations used in the Conditional Moment Closure methods.

3) The forward-time diffusion model does generally comply with theoretical expectations for a Markov model of this kind. However, the forward-time diffusion model underpredicts the rate of diffusion in velocity space, while the prediction for the rate of diffusion in scalar space is accurate. These diffusion rates affect predictions for the turbulent dispersion from a localized source.

4) The optimal diffusion model (i.e. the best model from the same class of models) largely coincides with the forward-time diffusion model, except for the coefficients B_{ij} determining the diffusion rate in the velocity space. These coefficients should be 3 to 10 times larger in the optimal model.

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