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CONDITIONAL METHODS AND LAGRANGIAN PARTICLE DIFFUSION

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ABSTRACT

Conditional methods are utilized for derivation of the Markov-type model for Lagrangian single-particle statistics of turbulent diffusion. This method gives theoretical prediction for the constant C_0 (the basic constant determining diffusion coefficient in velocity phase space). In traditional methods this constant is considered as an empirical constant.

INTRODUCTION

The main requirement for any model claiming to describe turbulent diffusion of the Lagrangian particles is consistency with Richardson's (1926) law and Kolmogorov (1941) theory of turbulence. Obukhov (1959) noted that the concept of a Markov process applied to diffusion in the velocity phase space is consistent with these restrictions and suggested describing the diffusion in the velocity phase space by the correspondent Fokker-Plank equation. Since that time this approach was discussed in many publications (Monin and Yaglom, 1975). Thomson (1987) and Pope (1987) investigated basic consistency principles related to Markov assumptions. A set of corrections to Markov assumptions is related to up-todate knowledge on small-scale turbulence [large but finite Re number (Sawford, 1991); intermittent nature of turbulence (Pope and Chen, 1990; Borgas and Sawford, 1994)]. Double-particle models were considered by Durbin (1980), Novikov (1989) and Thomson (1990). Lagrangian particles diffusion in near-wall turbulence is considered by Dreeben and Pope (1995). But all of these approaches follow similar scheme: 1)the Markov-process assumption (sometimes with certain corrections to this concept) for diffusion in the velocity phase space; 2)the Fokker-Plank equation with unknown coefficients is then *postulated*; 3)the coefficients are determined by theoretical consistency conditions (when this is possible), by agreement of the solutions and experimental data or specified in a way avoiding complications.

Our purpose here is to develop an alternative approach for single-particle characteristics based on utilization of the conditional expectations. This has some similarities with Conditional Moment Closure (CMC) suggested by Klimenko (1990, 1993, 1995) and Bilger (1991, 1993) (see also Li and Bilger, 1993; Klimenko, Bilger and Roomina, 1995). The basic difference between traditional and conditional approaches is that the main equation is not postulated but *derived* on the basis of transport (Navier-Stokes and scalar transport) equations. Then the equation obtained is closed using Markov-type assumptions identical to assumptions of the traditional methods. The conditional equation being a consequence of the transport equations contains additional information about the coefficients of the model.

The relation of the Lagrangian pdf P_L and conditional characteristics is given by the equation

$$P_L = \frac{1}{n_m} Q_u P_u \tag{1}$$

where $n_m = \langle n_c \rangle$ is the average total number of particles (which is assumed to be extremely large); c is their instantaneous concentration measured in particles per volume; density is assumed to be the constant ρ=const; $Q_u = Q_u(\mathbf{u}, \mathbf{x}, t) \equiv \langle c | \mathbf{u} \rangle$ is expectation conditioned on a fixed value of velocity and P_u is the Eulerian velocity pdf. The Lagrangian pdf $P_L = P_L(\mathbf{u}, \mathbf{x}, t)$ is introduced as the probability for one of the particles (any particle chosen with equal probability) having a certain velocity at a given physical location and time. Equation (1) reflects that the probability of obeying certain conditions for particle trajectory $x_p(t)$, $u_p(t)$ of a particle (namely $x_i - \Delta x_i < (x_p)_i < x_i + \Delta x_i$ and $u_i - \Delta u_i < (u_p)_i < u_i + \Delta u_i$ at moment t) is proportional to the average number of particles obeying those conditions. Particle sampling includes two stages: 1) choice of one of the particles and 2) choice of realization of the turbulent field. If P_L is transitional pdf, all of the particles positions must satisfy certain initial conditions.

Concentration c can be also treated as a continuous scalar obeying the scalar transport equation (again: provided the number of particles is large). The particles we consider are not necessarily fluid particles and can be involved in Brownian-type motion which is responsible for molecular diffusion (Dreeben and Pope, 1995).

EQUATION FOR CONDITIONAL MEAN

The unclosed equation for the conditional mean Q_u can be obtained using the joint velocity - concentration pdf $P_+(\mathbf{u},c;\mathbf{x},t)\equiv P_+(\mathbf{f};\mathbf{x},t)$ which is governed by the equation (see Pope, 1985)

$$\frac{\partial P_+}{\partial t} + \mathrm{div}\left(<\mathbf{u}|\mathbf{f}>P_+\right) + \frac{\partial^2 N_{ij} P_+}{\partial f_i \partial f_j} = - \frac{\partial <S_i^\circ|\mathbf{f}>P_+}{\partial f_i} \qquad (2)$$

where $f_i\equiv u_i$, $S_i^\circ \equiv - \dfrac{1}{\rho}\dfrac{\partial p}{\partial x_i}$ for $i=1,2,3$

and $f_4\equiv c$, $S_4^\circ \equiv W$

$N_{ij}\equiv <D(\nabla f_i \cdot \nabla f_j)|\mathbf{f}>$

Equation (2) is a direct consequence of the Navier-Stokes and scalar transport equations

$$\frac{\partial u_i}{\partial t} + \mathrm{div}\left(\mathbf{u}u_i\right) - \mathrm{div}\left(D\nabla u_i\right) = - \frac{1}{\rho}\frac{\partial p}{\partial x_i} \qquad (3)$$

$$\frac{\partial c}{\partial t} + \mathrm{div}\left(\mathbf{u}c\right) - \mathrm{div}\left(D\nabla c\right) = W \qquad (4)$$

The Re number is assumed to be high in Eq.(2) so molecular transport can be neglected (Kuznetsov and Sabelnikov, 1989). Another restriction: the diffusion coefficient D is taken to be equal to the viscosity coefficient ν so any effects related to $Sc\neq 1$ are not considered here. The joint pdf equation is multiplied by c and integrated over all possible concentrations c

$$\frac{\partial Q_u P_u}{\partial t} + \frac{\partial u_i Q_u P_u}{\partial x_i} + \frac{\partial}{\partial u_i} H_i = - \frac{\partial G_i Q_u P_u}{\partial u_i} + W_u P_u \qquad (5)$$

where $i=1,2,3$; $G_i\equiv - <\partial p/\partial x_i|\mathbf{u}>/\rho$; $S_i=-(\partial p/\partial x_i)/\rho$

and $$H_i = \frac{\partial <D(\nabla u_i \cdot \nabla u_j)c|\mathbf{u}>P_u}{\partial u_j} - 2<D(\nabla u_i \cdot \nabla c)|\mathbf{u}>P_u + <c''S_i''|\mathbf{u}>P_u \qquad (6)$$

is a flux of scalar c in velocity phase space; Eulerian velocity pdf P_u is governed by the equation

$$\frac{\partial P_u}{\partial t} + \frac{\partial u_i P_u}{\partial x_i} + \frac{\partial^2 \varepsilon_{ij} P_u}{\partial u_i \partial u_j} = - \frac{\partial G_i P_u}{\partial u_i} \qquad (7)$$

$\varepsilon_{ij} \equiv <D(\nabla u_i \cdot \nabla u_j)|\mathbf{u}>$ is dissipation tensor;
$(\cdot)'' \equiv (\cdot) - <(\cdot)|\mathbf{u}>$ denotes fluctuations with respect to conditional mean.

Eq.(5) can be written as the equation for Lagrangian pdf P_L

$$\frac{\partial P_L}{\partial t} + \frac{\partial u_u P_L}{\partial x_i} + \frac{\partial G_i P_L}{\partial u_i} + \frac{\partial}{\partial u_i}\frac{H_i}{n_m} = 0 \qquad (8)$$

In order to avoid complications we assume in Eq.(8) that $W=0$ and the average total number of particles n_m is a constant (particles do not appear or disappear). The instantaneous total number of particles n_c can be, however, different for different realizations (depending on initial conditions), but n_c=const for each of the realizations.

ANALOGY WITH MARKOV PROCESS

We consider a random process $u_p(t)$ where u_p is one of the components of particle velocity. According to Kolmogorov (1941) theory the increment of u_p is estimated as $<(\Delta u_p)^2>=C_0\varepsilon_m\Delta t$ where C_0 is a constant, ε_m is the mean dissipation of energy and Δt is time interval of the inertial interval of turbulence $t_k \ll \Delta t \ll t_L$. Here t_k is the Kolmogorov time scale and t_L is the time macroscale (Lagrangian). The correlation R of the particle accelerations $\dot{u}_p \equiv du_p/dt$ is given by

$$R(\Delta t) \equiv <\dot{u}_p(t_0+\Delta t)\,\dot{u}_p(t_0)> =$$
$$= \frac{1}{2}\frac{d^2}{dt^2} <(\Delta u_p)^2> = \frac{1}{2}\frac{d^2}{dt^2} C_0\varepsilon_m\Delta t = 0 \qquad (9)$$

That is Lagrangian accelerations are not correlated for $\Delta t \gg t_k$ and t_k is an estimation of the characteristic correlation time for accelerations. Obukhov (1959) assumed that this indicates an analogy of particle motions in the velocity phase space and Brownian motion (Markov process). The Markov assumption is not absolute: accelerations can be uncorrelated but, in strict mathematical sense, statistically dependent (this can be related to the internal intermittency phenomenon). We must also note that Eq.(9) is only the main order equation and correlation R may include weak but long-time correlations (Monin and Yaglom, 1975). In this paper we follow Obukhov's hypothesis and do not consider these corrections.

If $W\neq 0$, particles appear (for $W>0$) and disappear (for $W<0$). We can still consider such particles as Brownian provided the characteristic "life time" τ_p of the majority of the particles is much greater than the characteristic correlation time: $\tau_p \gg t_k$.

MARKOV-TYPE APPROXIMATION

Following Obukhov's (1959) hypothesis we approximate flux H_i by the diffusion approximation

$$\frac{H_i}{n_m} = A_i^\circ P_L - B_{ij}^\circ \frac{\partial P_L}{\partial u_j} \qquad (10)$$

with unknown drift A_i° and diffusion B_{ij}° coefficients. Equation (10) can be rewritten in terms of conditional means

$$H_i = A_i Q_u - B_{ij}\frac{\partial Q_u}{\partial u_j} \qquad (11)$$

where $A_i=A_i^\circ P_u - B_{ij}^\circ \dfrac{\partial P_u}{\partial u_j}$ and $B_{ij}=B_{ij}^\circ P_u$

Coefficients A_i° and B_{ij}° can be determined because they are restricted by some properties of the system (3)-(4).

1)If scalar c is passive, Eq.(4) is linear with respect to c. So that $c=ac_a+bc_b$, $W=aW_a+bW_b$ is solution of Eq.(4) with arbitrary constants a and b, provided c_a,W_a and c_b,W_b are also solutions of Eq.(4). This property can be formulated in terms of conditional means: $Q_u=aQ_{ua}+bQ_{ub}$, $W_u=aW_{ua}+bW_{ub}$ is a solution of Eq.(5) provided both Q_{ua},W_{ua} and Q_{ub},W_{ua} obey Eq.(5). The consequence is quite evident: if the diffusion approximation of H_i is correct (and we assume in this paper that it is correct) then coefficients A_i and B_{ij} must not depend on Q_u. It is possible now to determine A_i and B_{ij} for one particular Q_u and the coefficients must be the same for any other Q_u.

2)Since $W=0$, $c=c_0$=const is a solution of Eq.(4) then $W_u=0$, $Q_u=c_0$ must make an identity of Eq.(5). This (in combination with Eqs. (5), (7), (11) gives $A_i=\partial(\varepsilon_{ij}P_u)/\partial u_j+\psi_i$ where ψ_i is an arbitrary vector chosen so that $\partial\psi_i/\partial u_i=0$. Equation (6) yields $\psi_i=0$ for $c=c_0$.

3)Another property of the transport equations (3)-(4) is that if $W\rho=-a_i\partial p/\partial x_i$ (where a_i=const) then $c=a_iu_i+c_0$ is the solution of the equation (4). If we wish to avoid negative concentrations c, we choose value of the constant c_0 which is large enough (otherwise we put $c_0=0$). The conditional means are given by $Q_u=a_iu_i+c_0$ and $W_u=a_iG_i$ and these relations must be a solution of Eq.(5). Substituting $Q_u=a_iu_i+c_0$ and $W_u=a_iG_i$ into Eqs. (5), (7), (11) we obtain $B_{ij}=\varepsilon_{ij}P_u+\psi_{ij}$ where $\partial\psi_{ij}/\partial u_i=0$. Equation (6) requires that $\psi_{ij}=0$ for $c=a_iu_i+c_0$.

In order to ensure that the diffusion approximation (11) is applicable for this solution we should also determine if $\tau_p \gg t_k$. If $W<0$ in a microvolume (which smaller than Kolmogorov length scale x_k, but still containing a large number of particles), particles disappear from this microvolume. Within the time interval $\Delta t \ll t_k$ the value of $W=a_iG_i$ is not changed significantly. The number of particles that have disappeared is estimated as $\Delta c \sim c_k\Delta t/t_k \sim cu_k\Delta t/(ut_k)$ where subscript "k" is for the correspondent Kolmogorov scales and $\nabla p\sim\rho u_k/t_k$. The probability P_Δ of any of the particles to disappear within the Δt interval is given by $P_\Delta \sim \Delta c/c \sim u_k\Delta t/(ut_k) \sim \mathrm{Re}^{-1/4}\Delta t/t_k$ (particles which disappear are chosen with equal probability and independently for each Δt). So we must wait a longer time $\tau_p\sim\Delta t/P_\Delta$ to have a significant chance of disappearance of a chosen particle. The particle "life time" τ_p is estimated as $\tau_p\sim t_k\mathrm{Re}^{1/4}\gg t_k$.

The equation for flux H_i takes the form

$$H_i = -\varepsilon_{ij}P_u\frac{\partial Q_u}{\partial u_j} + \frac{\partial\varepsilon_{ij}P_u}{\partial u_j}Q_u \tag{12}$$

CONSISTENCY WITH KOLMOGOROV THEORY

By substituting closure (12) into equations (5) and (8) we obtain

$$\frac{\partial Q_uP_u}{\partial t} + \frac{\partial u_iQ_uP_u}{\partial x_i} - \varepsilon_{ij}P_u\frac{\partial^2 Q_u}{\partial u_i\partial u_j} + \frac{\partial^2\varepsilon_{ij}P_u}{\partial u_i\partial u_j}Q_u =$$

$$= -\frac{\partial G_iQ_uP_u}{\partial u_i} + W_uP_u \tag{13}$$

This equation contains inverse parabolic terms related to the Eulerian pdf equation (7) and direct parabolic terms related to the equation for the conditional mean Q_u

$$\frac{\partial Q_u}{\partial t} + u_i\frac{\partial Q_u}{\partial x_i} + G_i\frac{\partial Q_u}{\partial u_i} - \varepsilon_{ij}\frac{\partial^2 Q_u}{\partial u_i\partial u_j} = W_u \tag{14}$$

Equation (14) is obtained from Eq.(13) and Eq.(7). Equation (13) can be also written as the equation for the Lagrangian pdf (assuming that $W=0$)

$$\frac{\partial P_L}{\partial t} + \frac{\partial u_iP_L}{\partial x_i} + \frac{\partial G_i^\circ P_L}{\partial u_i} - \frac{\partial^2\varepsilon_{ij}P_L}{\partial u_i\partial u_j} = 0 \tag{15}$$

where

$$G_i^\circ = G_i + \frac{2}{P_u}\frac{\partial\varepsilon_{ij}P_u}{\partial u_j};\quad G_i \equiv -\frac{1}{\rho}\left\langle\frac{\partial p}{\partial x_i}\Big|\mathbf{u}\right\rangle \tag{16}$$

Equation (15) can be treated as a Fokker-Plank equation describing the correspondent Markov process.

Obukhov's original model implies that diffusion in velocity phase space is isotropic and that conventional (but not conditional) dissipation of energy is a determining parameter of this process. Equation (16) is consistent with the original model provided we apply those assumptions:

1)ε_{ij} does not depend on $\mathbf{u}$; that is $\varepsilon_{ij}=\langle D(\nabla u_i\cdot\nabla u_j)\rangle$;

2)local isotropy: $\varepsilon_{ij}=\varepsilon_m\delta_{ij}/3$ where ε_m is conventional average dissipation of energy

$$\varepsilon_m \equiv \left\langle\sum_{i,j}\frac{D}{2}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)^2\right\rangle = \left\langle D\left(\frac{\partial u_i}{\partial x_j}\frac{\partial u_i}{\partial x_j}\right)\right\rangle$$

Hence Eq.(15) takes the form

$$\frac{\partial P_L}{\partial t} + \frac{\partial u_iP_L}{\partial x_i} + \frac{\partial G_i^\circ P_L}{\partial u_i} - B_0\frac{\partial^2 P_L}{\partial u_i\partial u_i} = 0 \tag{17}$$

where the diffusion coefficient in velocity phase space is given by

$$2B_0 = C_0\varepsilon_m;\qquad C_0 = 2/3 \tag{18}$$

and

$$G_i^\circ = -\frac{1}{\rho}\left\langle\frac{\partial p}{\partial x_i}\Big|\mathbf{u}\right\rangle + \frac{2B_0}{P_u}\frac{\partial P_u}{\partial u_i} \tag{19}$$

The derived form of the drift coefficient G_i° provides consistency of Lagrangian and Eulerian pdfs. We note that $Q_u=c_0$=const, $W=0$ is a solution of Eq.(14). If $Q_u=c_0$ (and if V_0, the total volume of the flow, is finite), the Lagrangian pdf is given by $P_L=P_u/V_0$ (note $n_m=c_0V_0$ and Eq.(1)). Substitution of $P_L=P_u/V_0$ into Eq.(17) yields equation which is consistent with the Eulerian pdf equation (7).

Let us consider an energy balance for Eq.(17) in the case of homogeneous turbulence. Multiplying Eq.(17) by $k\equiv u^2/2$ and integrating we obtain

$$\frac{dk}{dt} + \langle G_i^\circ u_i\rangle_L = 3B_0 = \varepsilon_m \tag{20}$$

Here $\langle\cdot\rangle_L$ denotes averaging using the Lagrangian pdf P_L. If $P_L \to P_u$ (this corresponds to the Lagrangian - Eulerian consistency principle) then $\langle \overset{\circ}{G}_i u_i \rangle_L \to \langle \overset{\circ}{G}_i u_i \rangle = 2\varepsilon_m$ and Eq.(20) takes the form $dk/dt = -\varepsilon_m$ which specifies the Eulerian energy balance in homogeneous turbulence. We substitute P_u for P_L in Eq.(20) and note that pressure-velocity correlations do not affect k. Krasnoff and Peskin (1971) considered the Langevin model and arbitrarily assumed that if $P_L = P_u$ then $\langle \overset{\circ}{G}_i u_i \rangle_L$ represents the dissipation rate $\varepsilon_m = \langle \overset{\circ}{G}_i u_i \rangle_L$ (we express those assumptions in terms of the equations obtained here). Their next assumption is that $dk/dt=0$. It can be seen from Eq.(20) that the combination of $\langle \overset{\circ}{G}_i u_i \rangle_L \to \varepsilon_m$ and $dk/dt=0$ gives a similar value of $B_0 = \varepsilon_m/3$. Each of those estimations is different from that derived here but the errors compensate each other.

CONCLUSIONS

The conditional technique developed in this paper gives theoretical prediction for the constant C_0 determining diffusion coefficient in velocity phase space (this conditional method has some similarities with Conditional Moment Closure). The only assumptions we use are the assumptions of Obukhov's (1959) original model. The prediction of the constant is possible since the suggested derivation of the model utilizes the Navier-Stokes and scalar transport equations while traditional methods simply postulate a Fokker-Plank equation. We should note that recent Direct Numerical Simulation (DNS) results give larger values of $C_0 \approx 2 \div 4$ (Pope, 1987). The earlier measurements of the constants related to C_0 for atmospheric and ocean flows with large Re number have large scattering and some of them give estimations for C_0 smaller than that obtained here (Monin and Yaglom, 1975, p.567).

The value of $\overset{\circ}{G}_i$ is not determined by a closed formula as $\overset{\circ}{G}_i$ is not determined in conventional models. So different consistency requirements (Thompson, 1987; Pope, 1987; Sawford, 1993) must be implemented in order to specify $\overset{\circ}{G}_i$. The conditional method yields, however, unclosed equation (19) for $\overset{\circ}{G}_i$ and coefficient $\overset{\circ}{G}_i$ can be measured in experiments or determined from DNS data.

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REFERENCES

Bilger,R.W. (1991) "Conditional moment method for turbulent reacting flow using Crocco variable conditions", Charles Kolling Research Laboratory TNF-99, Dept. of Mech. Eng., The University of Sydney.

Bilger,R.W. (1993) "Conditional Moment Closure for Turbulent Reacting Flow", Phys. Fluids A, **5**, 436-444.

Borgas,M.S. and Sawford,B.L. (1994) "Stochastic equations with multifractal random increments for modeling turbulent dispersion", Phys.Fluids, **6**, 618-633.

Dreeben,T.D. and Pope,S.B. (1995) "PDF and Reynolds stress modeling of near-wall turbulent flows", 10th Symposium on Turbulent Shear Flows, V.1, p.2.1-2.6.

Durbin,P.A. (1980) "A stochastic model of two-particle dispersion and concentration fluctuations in homogeneous turbulence", J.Fluid Mech., **207**, 531-586.

Klimenko,A.Yu. (1990) "Multicomponent diffusion of various scalars in turbulent flow", Fluid Dyn., **25**, 327-334.

Klimenko,A.Yu. (1993) "Conditional moment closure and fluctuations of scalar dissipation", Fluid Dyn., **28**, 630-637.

Klimenko,A.Yu. (1995) "Note on the conditional moment closure in turbulent shear flows", Physics of Fluids, **7**, 446-448.

Klimenko,A.Yu., Bilger,R.W. and Roomina,M.R. (1995) "Some PDF Integrals for Self-Similar Turbulent Flows", Combust. Sci. and Tech. **107**, 4-6, p. 403.

Kolmogorov,A.N. (1941) "The local structure of turbulence in incompressible viscous fluid for very large Reynolds numbers", C.R.Acad.Sci. U.S.S.R., **30**, 301-305, No 4.

Krasnoff,E. and Peskin,R.L. (1971) "The Langevin model for turbulent diffusion", Geophysical Fluid Dyn., **2**, 123-146.

Kuznetsov,V.R. and Sabelnikov,V.A. (1989) Turbulence and Combustion, Hemisphere.

Li,J.D. and Bilger,R.W. (1993) "Measurements and prediction of the conditional variance in a turbulent reactive-scalar mixing layer," Phys. Fluids (A), **5**, 3255-3264.

Novikov,E.A.(1989), "Two-particle description of turbulence, Markov property and intermittency", Phys.Fluids A, **1**, 326-330.

Monin,A.S., Yaglom,A.M (1975) Statistical Fluid Mechanics. Volume 2, The Mit Press.

Obukhov,A.M. (1959) "Description of turbulence in terms of Lagrangian variables", Adv. Geophys., **6**, 113-116.

Pope,S.B. (1985) "PDF methods for turbulent reactive flows", Prog. Energ. Comb. Sci., **11**, 119-192.

Pope,S.B. (1987) "Consistency conditions for random-walk models of turbulent dispersion", Phys.Fluids, **30**, 2374-2379.

Pope,S.B. and Chen,Y.L. (1990) "The velocity - dissipation probability density function model for turbulent flows", Phys.Fluids A, **2**, 1437-1449.

Richardson,L.F. (1926) "Atmospheric diffusion shown on a distance-neighbor graph", Proc.Roy.Soc., **A110**, 709-737.

Sawford,B.L. (1991) "Reynolds number effects on Lagrangian statistic models of dispersion", Phys.Fluids A, **3**, 1577-1586.

Sawford,B.L. (1993) "Recent developments in the Lagrangian stochastic theory of turbulent dispersion", Bound.-Layer Meteor., **62**, 197-215.

Thomson,D.J. (1987) "Criteria for the selection of stochastic models of particle trajectories in turbulent flows", J.Fluid Mech., **180**, 529-556.

Thomson,D.J. (1990) "A stochastic model for the motion of particle pairs in isotropic high Re number turbulence", J.Fluid Mech., **207**, 113-153.