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On the one-point probability density function for the wind velocity in the neutral atmospheric surface layer

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The differential equation describing the one-point joint probability density function for the wind velocity given by Lundgren (1967) in neutral turbulent flows is extended by a term which also takes into consideration the pressure–mean strain interaction. For the new equation a solution is given describing the one-point probability density function for the wind velocity fluctuations if the profile of the mean wind velocity is logarithmic. The properties of this solution are discussed to identify the differences to a Gaussian having the same first and second moments.

1. Introduction

Studying turbulent dispersion with Lagrangian stochastic (LS) models requires more knowledge about the statistical properties of the underlying flow than only mean wind velocity components and variances. A turbulent flow is 'statistically known' on the lowest level from the viewpoint of using LS-models if the one-point probability density function is given (Thomson 1987).

Usually the probability density function is approximated by a probability density function maximizing the entropy under the condition that the moments to same order are given (Jaynes 1975). In this way the problem of determining the probability density function is reduced to the problem of estimating moments (e.g. Du, Wilson & Lee 1994).

The restriction to second moments yields the Gaussian probability density function as a maximum entropy approximation. For the atmospheric surface layer this approximation is widely used because the second moments are known for many cases from measurements (as discussed e.g. in Fiedler 1975) and also from calculations using equations for the second moments based on second-order closures (Mellor & Yamada 1982).

Deviations from a Gaussian probability density function characterized by third moments have been found in the full convective boundary layer (Willis & Deardorff, 1974). It was demonstrated (e.g. by Baerentsen & Berkowicz 1984) that these third moments are essential for the dispersion characteristics of the full convective boundary layer. It was also shown that for near-neutral atmospheric surface layers the fourth moments can play an important role in the dispersion problem (Heinz & Schaller 1996).

An alternative approach is to evaluate the probability density function directly by solving a partial differential equation for it. The governing equation for the one-point probability density distribution $f(1)$ (where $1 \equiv (v_k, x_k, t)$) of a turbulent, non-divergent, neutrally stratified flow was derived by Lundgren (1967):

$$\frac{\partial f(1)}{\partial t} + v_k \frac{\partial f(1)}{\partial x_k} + \left(-\frac{1}{\rho} \frac{\partial \overline{p}}{\partial x_k} - g_k + \nu \frac{\partial^2 V_k}{\partial x_j \partial x_j} \right) \frac{\partial f(1)}{\partial v_k} = \left.\frac{\partial f}{\partial t}\right|_p + \left.\frac{\partial f}{\partial t}\right|_f \tag{1.1}$$

with the mean velocity $V_k := \int v_k \; f(1) \; \mathrm{d}\boldsymbol{v}$, where the term

$$\left.\frac{\partial f}{\partial t}\right|_p = \frac{\partial}{\partial v_i} \left[\frac{1}{4\pi} \int \left(\frac{\partial}{\partial x_i} \frac{1}{r} \right) v_k^{(2)} v_l^{(2)} \frac{\partial^2 f'(1,2)}{\partial x_k^{(2)} \partial x_l^{(2)}} \mathrm{d}\boldsymbol{v}^{(2)} \mathrm{d}\boldsymbol{x}^{(2)} \right] \tag{1.2}$$

is responsible for the change of the probability density function $f(1)$ caused by pressure fluctuations ($\boldsymbol{r} = \boldsymbol{x}^{(2)} - \boldsymbol{x}$ and $2 \equiv (v_k^{(2)}, x_k^{(2)}, t)$). The term

$$\left.\frac{\partial f}{\partial t}\right|_f = -\frac{\partial}{\partial v_k} \lim_{x^2 \to x} \nu \frac{\partial^2}{\partial x_j^{(2)} \partial x_j^{(2)}} \left[\int v_k^{(2)} f'(1,2) \, \mathrm{d}\boldsymbol{v}^2 \right] \tag{1.3}$$

describes the change caused by friction forces. The function $f'(1,2)$ in these equations is defined as $f'(1,2) = f(1,2) - f(1) f(2)$. Both terms (equations (1.2) and (1.3)) are dependent on the two-point probability density function $f(1,2)$. For them it was shown by Lundgren (1967) that an equation similar to (1.1) can be found, depending on the three-point probability density function and so on.

Restricting ourselves to the one-point probability density function $f(1)$, approximations of the terms (1.2) and (1.3) are necessary. It was proposed by Lundgren (1969) that the term (1.3) is well approximated by the expression

$$\left.\frac{\partial f}{\partial t}\right|_f = \frac{1}{\gamma\tau} \frac{\partial}{\partial v_k} \left[(v_k - V_k) f(1) \right]. \tag{1.4}$$

Taking into consideration that terms of the kind

$$\left.\frac{\partial f}{\partial t}\right|_f = -\frac{\partial}{\partial v_k} \left[b_k f(1) \right]$$

are caused by forces $b_k(v_i, x_i)$ acting on a fluid particle moving with the velocity v_i at the point x_i, approximation (1.4) results from the assumption that the turbulent friction force acting on a fluid lump moving with the velocity v_i is proportional to the velocity difference $v_k - V_k$ to the environment moving with the mean wind velocity. This friction force is the turbulent analogy to the friction force acting on a moving sphere in a viscid fluid.

In Lundgren (1969) the term (1.2) was approximated by a relaxation term

$$\left.\frac{\partial f}{\partial t}\right|_p = -\frac{f(1) - f_0(1)}{\tau}, \tag{1.5}$$

where τ is the relaxation time and the 'equilibrium' probability density function f_0 is assumed to be an isotropic Gaussian

$$f_0(1) = \left(2\pi \tfrac{2}{3} E\right)^{-3/2} \exp\left(-\frac{1}{2} \frac{(v_i - V_i)(v_i - V_i)}{\tfrac{2}{3}E} \right) \tag{1.6}$$

characterized by the turbulent kinetic energy E.

From equation (1.1) with the approximations (1.4) and (1.5) equations for the second moments may be derived (e.g. Kurbazkii 1988). These second-moments equations demonstrate that approximation (1.5) leads to the expression from Rotta (1951) for the pressure–strain correlations caused by the wind velocity fluctuations. Also it can be seen from these equations that there is no term modelling the pressure–strain interaction caused by mean strain rates included in the approximation (1.5). It is known that neglecting this interaction may cause unsatisfactory results in turbulent shear flows. Even in the case of a simple one-dimensional homogeneous shear flow equation (1.1) with the approximations (1.4) and (1.5) predicts that the variance of both wind velocity components perpendicular to the mean wind velocity is equal (e.g. Kurbazkii 1988) which is in contradiction to variances of the wind velocity measured in plane homogeneous shear layers where the wind velocity variance in the direction of the shear is smaller than the variance of the wind velocity perpendicular to the direction of shear and to the direction of the mean wind velocity.

To overcome these difficulties we introduce an approximation of the term (1.2) similar to Pope (1985) taking into account also the pressure–strain interaction caused by the mean shear.

The modified Lundgren (1969) equation for the one-point probability density function is then solved for the special case of a neutral atmospheric surface layer characterized by a logarithmic wind profile.

Some properties of this solution are discussed in the framework of identifying the deviations from a Gaussian probability density function.

2. Pressure–strain interaction

The term (1.2) may be split-up into a pressure–diffusion and a pressure–strain interaction term

$$\left.\frac{\partial f}{\partial t}\right|_p = \left.\frac{\partial f}{\partial t}\right|_D + \left.\frac{\partial f}{\partial t}\right|_P,$$

where the diffusion term is

$$\left.\frac{\partial f}{\partial t}\right|_D = \frac{\partial}{\partial x_i}\frac{\partial}{\partial v_i}\left[\frac{1}{4\pi}\int \frac{1}{r}v_k^{(2)}v_l^{(2)}\frac{\partial^2 f'(1,2)}{\partial x_k^{(2)}\partial x_l^{(2)}}\mathrm{d}\boldsymbol{x}^{(2)}\mathrm{d}\boldsymbol{v}^{(2)}\right]$$

and the pressure–strain interaction term is

$$\left.\frac{\partial f}{\partial t}\right|_P = -\frac{\partial}{\partial v_i}\left[\frac{1}{4\pi}\int \frac{1}{r}v_k^{(2)}v_l^{(2)}\frac{\partial^3 f'(1,2)}{\partial x_i\partial x_k^{(2)}\partial x_l^{(2)}}\mathrm{d}\boldsymbol{x}^{(2)}\mathrm{d}\boldsymbol{v}^{(2)}\right]. \tag{2.1}$$

In the following we will restrict ourselves to the second part $\partial f/\partial t|_P$ because the pressure diffusion is of minor interest in many types of turbulent flows (Kurbazkii 1988).

Introducing the new coordinates $\boldsymbol{r} = \boldsymbol{x} - \boldsymbol{x}^{(2)}$, $\boldsymbol{u} = \boldsymbol{v} - \boldsymbol{V}$ and $\boldsymbol{u}^{(2)} = \boldsymbol{v}^{(2)} - \boldsymbol{V}^{(2)}$ equation (2.1) is written as

$$\left.\frac{\partial f}{\partial t}\right|_P = -\frac{\partial}{\partial u_i}\left[\frac{1}{4\pi}\int\left(\frac{\partial^2 r^{-1}}{\partial r_k\partial r_l}\right)v_k^{(2)}v_l^{(2)}g_i(1,2)\,\mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{u}^{(2)}\right] \tag{2.2}$$

with

$$g_i(1,2) = \frac{\partial f'(1,2)}{\partial x_i} - \frac{\partial f'(1,2)}{\partial r_i} - \frac{\partial f'(1,2)}{\partial u_m^{(2)}}\frac{\partial V_m^{(2)}}{\partial x_i^{(2)}} - \frac{\partial f'(1,2)}{\partial u_m}\frac{\partial V_m}{\partial x_i}.$$

Assuming local homogeneity, the function $f'(1,2)$ written in the new coordinates is independent of x_i. Assuming further that the shear $\partial V_m/\partial x_i$ is constant yields

$$g_i(1,2) = -\frac{\partial f'(1,2)}{\partial r_i} - \left(\frac{\partial f'(1,2)}{\partial u_m^{(2)}} + \frac{\partial f'(1,2)}{\partial u_m}\right)\frac{\partial V_m}{\partial x_i}.$$

Inserting this expression into equation (2.2), after rearranging the terms and taking into account the divergence condition for the two-point probability density function given by Lundgren (1969)

$$\frac{\partial}{\partial r_i}\int u_i^{(2)} f(1,2)\,\mathrm{d}\boldsymbol{u}^{(2)} = \frac{\partial}{\partial r_i}\int u_i f(1,2)\,\mathrm{d}\boldsymbol{u} = 0,$$

yields

$$\begin{aligned}\left.\frac{\partial f}{\partial t}\right|_P = &-\frac{\partial}{\partial u_i}\left[\frac{1}{4\pi}\int \frac{\partial^3 r^{-1}}{\partial r_i \partial r_l \partial r_k} u_k^{(2)} u_l^{(2)} f'(1,2)\,\mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{u}^{(2)}\right]\\ &+\frac{\partial V_k}{\partial x_l}\frac{\partial}{\partial u_i}\left[\frac{1}{2\pi}\int \frac{\partial^2 r^{-1}}{\partial r_i \partial r_k} u_l^{(2)} f'(1,2)\,\mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{u}^{(2)}\right]\\ &+\frac{\partial V_m}{\partial x_i}\frac{\partial^2}{\partial u_i \partial u_m}\left[\frac{1}{4\pi}\int \frac{\partial^2 r^{-1}}{\partial r_k \partial r_l} v_k^{(2)} v_l^{(2)} f'(1,2)\,\mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{u}^{(2)}\right].\end{aligned} \tag{2.3}$$

The first term in this equation is the only non-vanishing term in the absence of shear and can be approximated (see Appendix A) by the relaxation term (1.5).

It can be shown that, unlike the other terms, the last one is not participating in the redistribution of the second moments. Assuming only weak shear, by neglecting the parts proportional to the square of shear, the last term is responsible for the interaction between deviations of the probability density function from a Gaussian and shear, because the term vanishes if the probability density function is a Gaussian. The first and the second terms only vanish if the probability density function is an isotropic Gaussian and give a reason for changing the probability density function only if there is a deviation from the Gaussian. Compared to deviations from an isotropic Gaussian we will assume that the deviations from a Gaussian are small so that we can neglect completely the last term compared to the first and second ones.

The second term in equation (2.3) is responsible for the interaction between shear and the deviation of the probability density function from an isotropic Gaussian. An approximation of this term can be found in the following way. Using

$$U_k^{(2)}(u_i, r_i) = \int u_k^{(2)} \frac{f(1,2)}{f(1)}\mathrm{d}\boldsymbol{u}^{(2)}$$

for the conditional mean value of the wind velocity, the second term on the right-hand side of equation (2.3) (hereafter denoted $\partial f/\partial t|_{P_2}$) may be written as (Pope 1985)

$$\left.\frac{\partial f}{\partial t}\right|_{P_2} = \frac{\partial V_k}{\partial x_l}\frac{\partial}{\partial u_i} f(1)\left[\frac{1}{2\pi}\int \frac{\partial^2 r^{-1}}{\partial r_i \partial r_k} U_l^{(2)}(u_i, r_i)\,\mathrm{d}\boldsymbol{r}\right].$$

Assuming the probability density function is a Gaussian one the conditional mean is

$$U_l^2(u_i, r_i) = R_{lm}^{(2,1)} R_{mj}^{-1} u_j, \tag{2.4}$$

where we took for the two-point velocity correlation tensor $R_{lm}^{(2,1)} = \overline{u_l^{(2)} u_m}$ and

$$\left.\frac{\partial f}{\partial t}\right|_{P_2} = -\frac{\partial}{\partial u_i}\frac{\partial V_k}{\partial x_l} a_{ik}^{ml} R_{mn}^{-1} u_n f(1) \tag{2.5}$$

with

$$a_{ik}^{ml} = -\frac{1}{2\pi} \int \frac{\partial^2 r^{-1}}{\partial r_i \partial r_k} R_{lm}^{(2,1)} \mathrm{d}\boldsymbol{r}. \tag{2.6}$$

Expression (2.5) was proposed by Pope (1985) for the second term in equation (2.3). The coefficients $a_{ik}^{ml} R_{ms}^{-1}$ in this ansatz are nonlinear in R_{ij} if one is assuming the expression for the tensor a_{ik}^{ml} given by Launder, Reece & Rodi (1975). Using once again the assumption that the probability density function is a Gaussian results in

$$\left.\frac{\partial f}{\partial t}\right|_{P_2} = \frac{\partial f(1)}{\partial u_i \partial u_m} \frac{\partial V_k}{\partial x_l} a_{ik}^{ml}. \tag{2.7}$$

The coefficients in this ansatz are now linear in R_{ij}. At this point we should also state that this term is not a diffusion term, because the matrix of coefficients is not positive definite in all cases. Similar to the assumption made by Lundgren (1969) to get an approximation of the friction term (1.4) we will presume that equation (2.4), which is exact for a Gaussian, is also a good approximation for probability density functions deviating only a little from Gaussian. Calculating the second-moment equation with the term (2.7) shows that it leads to the redistribution of the second moments caused by pressure–mean strain interaction. From equation (2.6) some symmetry relations for the tensor a_{lj}^{mi} can be derived which lead in common with a linear ansatz in the Reynolds stresses to the representation given by Launder *et al.* (1975)

$$\begin{aligned} a_{lj}^{mi} = {} & \alpha \delta_{lj} R_{im} + \beta(\delta_{ml} R_{ij} + \delta_{mj} R_{il} + \delta_{il} R_{jm} + \delta_{ij} R_{ml}) \\ & + c_2 \delta_{mi} R_{jl} + \left(\eta \delta_{mi} \delta_{lj} + \nu(\delta_{ml}\delta_{ij} + \delta_{mj}\delta_{il})\right) \frac{R_{pp}}{2} \end{aligned} \tag{2.8}$$

with constants

$$\alpha = \frac{4c_2 + 10}{11}, \qquad \beta = -\frac{3c_2 + 2}{11}, \qquad \eta = -\frac{50c_2 + 4}{55}, \qquad \nu = \frac{20c_2 + 6}{55}. \tag{2.9}$$

With this approximation (back transformed to v_k) the final form of equation (1.1) for the probability density function is

$$\begin{aligned} & \frac{\partial f(1)}{\partial t} + v_k \frac{\partial f(1)}{\partial x_k} + \left(-\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_k} - g_k + \nu \frac{\partial^2 V_k}{\partial x_j \partial x_j}\right) \frac{\partial f(1)}{\partial v_k} - \frac{1}{\gamma\tau}\frac{\partial}{\partial v_k}\left[(v_k - V_k) f(1)\right] \\ & \qquad = \frac{f_0(1) - f(1)}{\tau} + \frac{\partial f(1)}{\partial v_i \partial v_m} \frac{\partial V_k}{\partial x_l} a_{ik}^{ml}. \end{aligned} \tag{2.10}$$

3. Calculation of the distribution function

One possible way of solving equation (2.10) is to presume a mean wind velocity distribution $\boldsymbol{V}(\boldsymbol{x}, t)$ and to look for an adequate distribution function. Transformation of the velocity $\boldsymbol{u} := \boldsymbol{v} - \boldsymbol{V}(\boldsymbol{x}, t)$ and transition to a new distribution function $f(\boldsymbol{u} + \boldsymbol{V}, \boldsymbol{x}, t) \rightarrow f(\boldsymbol{u}, \boldsymbol{x}, t)$ in (2.10) yield

$$\begin{aligned} & \frac{\partial f}{\partial t} - \frac{\partial V_k}{\partial t}\frac{\partial f}{\partial u_k} + (u_k + V_k)\left(\frac{\partial f}{\partial x_k} - \frac{\partial V_l}{\partial x_k}\frac{\partial f}{\partial u_l}\right) + \left(-\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_k} - g_k + \nu\frac{\partial^2 V_k}{\partial x_j \partial x_j}\right)\frac{\partial f}{\partial v_k} \\ & \qquad - \frac{1}{\gamma\tau}\frac{\partial}{\partial u_k}(u_k f) = \frac{f_0 - f}{\tau} + \frac{\partial^2 f}{\partial u_i \partial u_j}\frac{\partial V_k}{\partial x_l} a_{ik}^{jl}. \end{aligned} \tag{3.1}$$

Solutions have to fulfil two consistence conditions: the normalization condition

$$1 = \int f(\boldsymbol{u}, \boldsymbol{x}, t) \mathrm{d}\boldsymbol{u} \tag{3.2}$$

and the condition of a vanishing averaged velocity deviation

$$0 = \int u_k \, f(\boldsymbol{u}, \boldsymbol{x}, t) \mathrm{d}\boldsymbol{u}. \tag{3.3}$$

Now we consider a horizontally homogeneous and stationary turbulent shear flow. Therefore we neglect the pressure gradient and gravity. Also the viscous term on the left-hand side of (3.1) is neglected (Lundgren 1969). The continuity equation for incompressible media yields $\boldsymbol{V}(z) = (U(z), 0, 0)$ and equation (3.1) simplifies to

$$u_3 \left(\tau \frac{\partial f}{\partial z} - \left(\tau \frac{\partial U}{\partial z} \right) \frac{\partial f}{\partial u_1} \right) - \frac{1}{\gamma} \frac{\partial}{\partial u_k} (u_k f) = (f_0 - f) + \frac{\partial^2 f}{\partial u_i \partial u_j} \left(\tau \frac{\partial U}{\partial z} \right) a_{1j}^{3i}(z).$$

We make the further assumption that the probability density function f is independent of height

$$\frac{\partial f}{\partial z} = 0.$$

From this follows that all the coefficients have to be independent of z. The equality $\tau \partial U / \partial z = \text{const} = G/\gamma$ means that the gradient of the averaged velocity is the reciprocal of the relaxation time and yields the well known logarithmic profile if $\tau \sim z$. If the tensor components a_{1j}^{3i} are independent of z, all the Reynolds stresses are independent of z too. All these additional assumptions result finally in the PDE

$$-u_3 G \frac{\partial f}{\partial u_1} - \frac{\partial}{\partial u_l} (u_l f) = \gamma (f_0 - f) + \frac{\partial^2 f}{\partial u_j \partial u_l} G \, a_{1l}^{3j} \tag{3.4}$$

with constant coefficients γ, G and a_{1l}^{3j} (see Launder *et al.* 1975 or equations (2.8), (2.9)). It can be changed to a PDE of first order by Fourier transformation

$$F(\boldsymbol{k}) := \int f(\boldsymbol{u}) \, \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{u}} \, \mathrm{d}\boldsymbol{u}.$$

This yields

$$G \frac{\partial}{\partial k_3} (k_1 F) + k_l \frac{\partial F}{\partial k_l} = \gamma (F_0 - F) - k_j k_l F \, G \, a_{1l}^{3j} \tag{3.5}$$

with the Fourier transform of the Gaussian equilibrium function

$$F_0(\boldsymbol{k}) = \exp\left(-\tfrac{1}{2} \left(\tfrac{2}{3} E \right) k_l k_l \right).$$

The solution of this equation is (see appendix B for the steps to get this solution)

$$F(\boldsymbol{k}) = \gamma \int_0^1 \xi^{\gamma - 1} \exp\left(-\tfrac{1}{2} k_i N_{ij}(\xi) k_j \right) \mathrm{d}\xi \tag{3.6}$$

with the symmetric matrices $N_{ij}(\xi)$ defined as

$$N_{ij}(\xi) := -2 M_{ij}(\xi) + \tfrac{2}{3} E \xi^2 \begin{pmatrix} 1 + G^2 (\ln \xi)^2 & 0 & G \ln \xi \\ 0 & 1 & 0 \\ G \ln \xi & 0 & 1 \end{pmatrix}, \tag{3.7}$$

where the matrix $M_{ij}(\xi)$ gives the influence of pressure–mean strain interaction on the probability density function

$$
\begin{aligned}
M_{11} &= \frac{G^3}{2} a_{13}^{33} \xi^2 (\ln \xi)^2 + GA\xi^2 \ln \xi + \frac{G}{2} \left(a_{11}^{31} - A\right) (\xi^2 - 1), \\
M_{12} &= 0, \\
M_{13} &= G^2 a_{13}^{33} \xi^2 \ln \xi + A(\xi^2 - 1), \\
M_{22} &= \left(\tfrac{3}{11} c_2 + \tfrac{2}{11}\right) (\xi^2 - 1) E, \\
M_{23} &= 0, \\
M_{33} &= \left(-\tfrac{5}{11} c_2 + \tfrac{4}{11}\right) \left(\xi^2 - 1\right) E, \\
A &= \frac{G}{2}(a_{11}^{33} + a_{13}^{31}) - \frac{G^2}{2} a_{13}^{33}.
\end{aligned}
$$

The matrix $\boldsymbol{M}$ contains the Reynolds stresses, which are calculated commonly with G in the next paragraph.

The Fourier back transformation into the velocity domain yields finally the probability density function

$$
f(\boldsymbol{u}) = \frac{\gamma}{(2\pi)^{3/2}} \int_0^1 \frac{\xi^{\gamma-1}}{(\det \boldsymbol{N}(\xi)^{1/2})} \exp\left(-\tfrac{1}{2} u_j N_{j,l}^{-1}(\xi) u_l\right) \, \mathrm{d}\xi. \tag{3.8}
$$

It can be seen that this probability density function consists of a 'sum' of Gaussians having different second moments. This concept has already been used by other authors (e.g. Baerentsen & Berkowicz 1984) to specify the probability density function for the vertical wind velocity in the convective boundary layer. The difference is that they used a discrete approximation of (3.8) by two Gaussians having different expectation values.

4. Discussion

4.1. *The moments of the distribution function*

One advantage in considering the probability density function is that it contains all the one-point correlation functions. All of these moments are symmetric in all of their indices. So the second moments have 6 independent components, the third moments have 10 and the fourth moments have 15. For our problem there are in principle two distinct ways for calculating these moments.

The first way is to derive an equation for them from (3.4) or (3.5). For the second moments e.g. this can be done by applying the operator $\partial^2/(\partial k_m \partial k_n)$ on equation (3.5) and then setting $\boldsymbol{k} = 0$. The second way is to calculate the moments directly from the probability density function (3.8). This is easily done for the characteristic function (3.6) with aid of the moment theorem for the nth moment

$$
R_{j_1 \ldots j_n} := \overline{u_{j_1} \ldots u_{j_n}} = \frac{1}{i^n} \left. \frac{\partial^n F}{\partial k_{j_1} \ldots \partial k_{j_n}} \right|_{\boldsymbol{k}=0}.
$$

In particular one can find that with the zeroth moment

$$
F(\boldsymbol{k} = 0) = \gamma \int_0^1 \xi^{\gamma-1} \, \mathrm{d}\xi = 1
$$

	$R_{1,1}/E - 2/3$	$R_{2,2}/E - 2/3$	$R_{3,3}/E - 2/3$	$R_{1,3}/E$
Kader & Yaglom (1990)	0.376	0.006	−0.382	−0.182
Panofsky & Dutton (1984)	0.486	−0.037	−0.448	−0.218
$\gamma = 0.1; c_2 = 0.6$	0.437	0.023	−0.462	−0.227

TABLE 1. Comparison between measured and evaluated second moments

and the first moment

$$\left.\frac{\partial F}{\partial k_m}\right|_{\boldsymbol{k}} = 0 = k_m(\ldots)|_{\boldsymbol{k}=0} = 0$$

the two consistency conditions are fulfilled.

The first way for the second moments results in

$$G(\delta_{1m}R_{3n} + \delta_{1n}R_{3m}) + (2+\gamma)R_{mn} = \gamma\tfrac{2}{3}E\delta_{mn} + G(a^{3m}_{1n} + a^{3n}_{1m}).$$

Expressing E and a^{mi}_{jl} with equations (2.8), (2.9) by the Reynolds stresses R_{ij} yields a homogeneous system of linear equations of the form

$$C_{mn,ij}\, R_{ij} = 0.$$

The solvability condition $\det \boldsymbol{C} = 0$ yields an equation of fourth order for G dependent on the constants γ and c_2. The only reasonable solution is

$$G = \frac{(330)^{1/2}}{2}\frac{\gamma+2}{(11\gamma - 15c_2^2 - 30c_2 + 27)^{1/2}}.$$

Solving the linear system gives for the Reynolds stress tensor

$$\frac{R_{i,j}}{E} = \begin{bmatrix} \frac{2}{33}\,\frac{12c_2 + 11\gamma + 30}{\gamma+2} & 0 & \frac{R_{1,3}}{E} \\ 0 & \frac{2}{33}\,\frac{18c_2 + 11\gamma + 12}{\gamma+2} & 0 \\ \frac{R_{1,3}}{E} & 0 & -\frac{2}{33}\,\frac{30c_2 - 11\gamma - 24}{\gamma+2} \end{bmatrix}$$

and

$$\frac{R_{1,3}}{E} = -\frac{2\,(11\gamma - 15c_2^2 - 30c_2 + 27)^{1/2}\sqrt{330}}{165\;(\gamma+2)}.$$

These moments can be compared with measurements to estimate the numerical values of γ and c_2. It can be seen (table 1) that the choice $\gamma = 0.1$ and $c_2 = 0.6$ gives satisfactory results for second moments compared to the values for the moments recommended by Panofsky & Dutton (1984) for the atmospheric surface layer. The values proposed by Kader & Yaglom (1990) as characteristic for laboratory measurements show smaller deviations from the isotropic tensor for the second moments; nevertheless the overall agreement is quite good. Note that we used constants which are different from the values $c_2 = 0.4$ and $c_1 = 1.5$ which gives $\gamma = 2\,(c_1 - 1) = 1$ proposed by Launder *et al.* (1975) because we found better agreement for the atmospheric surface layer.

For the higher moments the second way is more convenient. For the third moments

$ijkl$	$\dfrac{R_{ijkl}}{E}$	$\dfrac{R^{(Gauss)}_{ijkl}}{E}$	$\left\lvert \dfrac{R_{ijkl} - R^{(Gauss)}_{ijkl}}{R^{(Gauss)}_{ijkl}} \right\rvert$
1111	9.727	3.665	1.654
1113	−1.458	−0.754	0.935
1122	0.761	0.762	0.002
1133	0.438	0.330	0.328
1223	−0.156	−0.157	0.003
1333	−0.166	−0.497	0.185
2222	1.427	1.427	0.000
2233	0.141	0.141	0.002
3333	0.142	0.126	0.124

TABLE 2. Non-zero values of the fourth moments

it follows in the same manner as for the first moments that

$$R_{lmn} = 0.$$

This is a little astonishing on one hand, because F is not isotropic (for an isotropic, symmetric tensor would it be trivial). On the other hand it is common to assume that third moments are proportional to gradients of the second moments (e.g. Kurbazkii 1988) and in our case the second moments are constant so that we could expect from this viewpoint vanishing third moments.

Consequently, the fourth moments should be considered. In particular, one should compare them with a Gaussian distribution with the same second moments, whose fourth moments can be expressed by

$$R^{(Gauss)}_{iklm} = R_{ik}R_{lm} + R_{il}R_{km} + R_{im}R_{kl}.$$

The fourth moments of f can be calculated as

$$R_{klmn} = \gamma \int_0^1 \xi^{\gamma-1} \; (N_{kl}N_{mn} + N_{km}N_{ln} + N_{kn}N_{lm}) \; \mathrm{d}\xi.$$

This integral can be calculated analytically, but is very confusing expressed by γ and c_2. But one can see by this form that from vanishing of the matrix elements N_{12}, N_{21}, N_{23}, N_{32} it follows that the moments R_{1112}, R_{1123}, R_{1222}, R_{1233}, R_{2222}, R_{2333} all are zero (as for the Gaussian distribution). Therefore, from the 81 tensor components only 9 are non-trivially independent. Their numerical values for $\gamma = 0.1$ and $c_2 = 0.6$ are given in table 2. It can be seen, that remarkable deviations from a Gaussian can be found only in the $f_{u,w}$ probability density function and especially in the f_u probability density function. We will discuss these features in the following.

4.2. *Marginal probability density functions*

Studying the one- or two-dimensional problem in the dispersion of air pollutants knowledge of the f_w and $f_{u,w}$ probability density function is necessary.

The characteristic function F_w for the f_w function is equal to $F(0, 0, k_3)$ where F is the characteristic function given by equation (3.6). Back transformation yields

$$f_w = \gamma \int_0^1 \xi^{\gamma-1} \frac{1}{(2\pi N_{3,3}(\xi))^{1/2}} \exp\left(-\tfrac{1}{2}\frac{w^2}{N_{3,3}(\xi)}\right) \mathrm{d}\xi, \tag{4.1}$$

where $N_{3,3}$ is the matrix component defined in (3.7). Comparing the probability

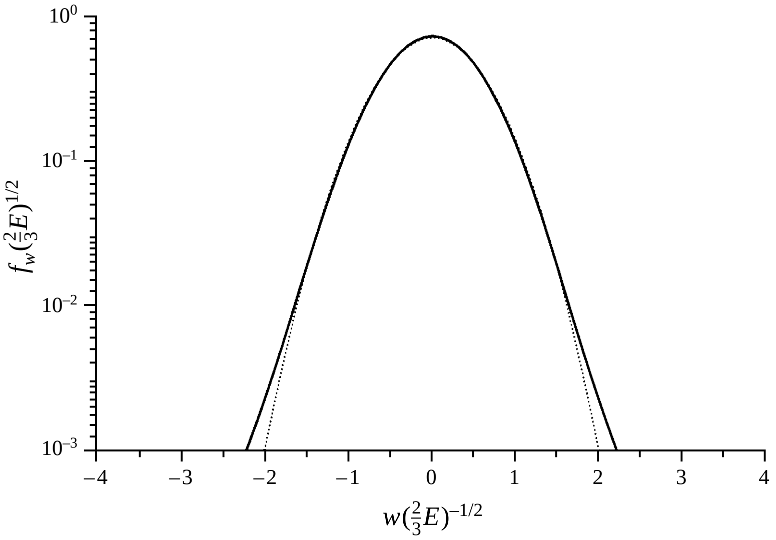

FIGURE 1. Probability density function f_w (solid line) compared to a Gaussian having the same variance (dotted line).

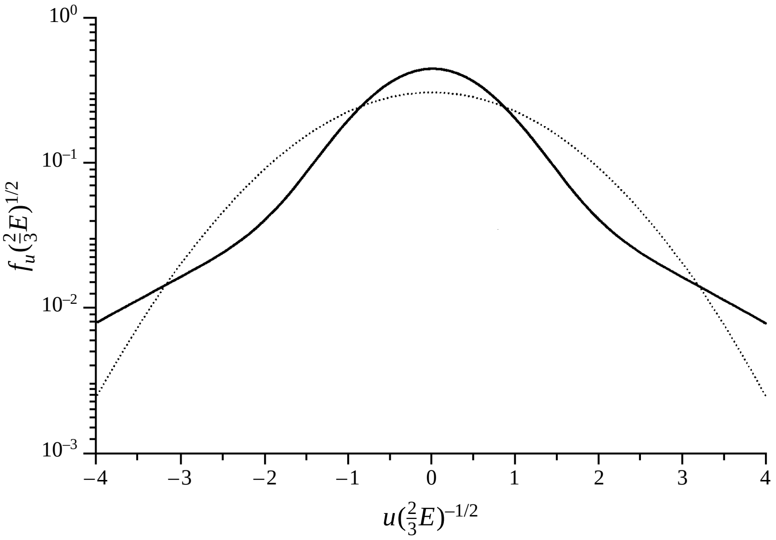

FIGURE 2. Probability density function f_u (solid line) compared to a Gaussian having the same variance (dotted line).

density function f_w with a Gaussian having the same standard deviation for the wind velocity component w, it can be seen (figure 1) that large wind velocity values are more frequent. This behaviour is characteristic of probability density functions having a positive excess, as found to be the case for the f_w distribution given above. In comparison to f_w, the f_u distribution

$$f_u = \gamma \int_0^1 \xi^{\gamma-1} \frac{1}{(2\pi N_{1,1}(\xi))^{1/2}} \exp\left(-\frac{1}{2}\frac{u^2}{N_{1,1}(\xi)}\right) \mathrm{d}\xi$$

is characterized by a greater kurtosis (figure 2).

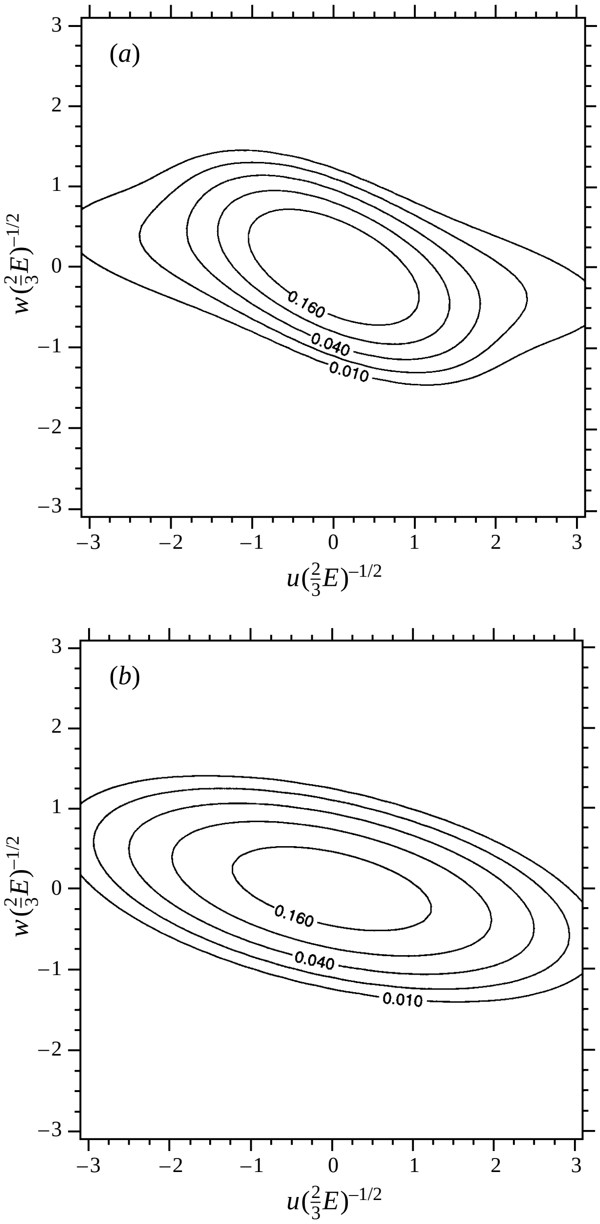

FIGURE 3. (*a*) $f_{u,w}$ probability density function and (*b*) Gaussian having the same second moments.

Analoguous to the above, the two-dimensional characteristic function is $F_{u,w} = F(k_1, 0, k_3)$. Using Greek indices with $(\alpha = 1, 3)$ the back transformation yields

$$f_{u,w} = \gamma \int_0^1 \xi^{\gamma-1} \frac{1}{2\pi(\det(N_{\alpha,\beta}(\xi))^{1/2}} \exp\left(-\tfrac{1}{2} u_\alpha N^{-1}_{\alpha,\beta}(\xi) u_\beta\right) \mathrm{d}\xi. \tag{4.2}$$

The stronger concentration of the wind velocity values around zero shown for the f_u and less significantly also for the f_w probability density function compared to an equivalent Gaussian is also visible in the $f_{u,w}$ distribution shown in figure 3. Another feature visible in figure 3 is the deviation from the ellipsoid shape of the isolines for the probability density at large wind velocity values.

Deviations from the Gaussian discussed before are dependent on the choice of our model parameters γ and c_1 typical for the turbulent surface layer of the atmosphere. Using the constants given by Launder *et al.* (1975) for laboratory turbulent shear flows results in much smaller deviations from a Gaussian.

5. Conclusions

The equation of Lundgren (1969) for the determination of the one-point probability density function was extended by an additional term to take into account also the mean shear–pressure fluctuation interaction. The resulting equation for the probability density yields the second moments equations used by Launder *et al.* (1975).

For the special case of a logarithmic boundary layer a solution of the resulting equation for the probability density function and also the characteristic function could be given.

By investigation of the fourth moments and the marginal probability density functions f_w, f_u and $f_{u,w}$ resulting from this solution it could be shown that the probability density function for the u-component is characterized by remarkable kurtosis, whereas the probability density function for the w-component, which is only produced by redistribution of the other components, has no remarkable kurtosis.

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Appendix A. The relaxation term

In our article we concentrate on some additional terms in the Lundgren (1969) equation for the one-point probability density function taking into account also the pressure–mean strain interaction. A problem left open is the question of whether the Boltzmann-type ansatz (1.5) for the first term in equation (2.3) proposed by Lundgren (1969) is appropriate or not.

Describing turbulent flows on the level of the one-point probability density function $f(1)$ can only be done by assuming the two-point probability density function $f(1,2)$ to be a functional of the one-point probability density function. In particular, the first term in equation (2.3) can be rewritten as a functional of $f(1)$, simply denoted as $P_1[f(u_i))]$. Expanding this nonlinear functional in a Taylor series around the isotropic Gaussian ‘equilibrium’ function (1.6) and taking into account only functionals linear in $f(1) - f_0(1)$ results in

$$P_1[f(u_i)] = P_1[f_0(u_i)] + \int \left. \frac{\delta P_1[f(u_i)]}{\delta f(u_i')} \right|_{f_0} \left(f(u_i') - f_0(u_i') \right) \mathrm{d}\boldsymbol{u}'. \qquad (\mathrm{A}\,1)$$

Using this approximation in equation (2.10) and assuming the isotropic Gaussian to be a solution of this equation under shear-free isotropic conditions the first term must be zero. The Boltzmann term proposed by Lundgren (1969) for the first term in (2.3) can be found from the approximation (A 1) as the first term in the Kramers–Moyal expansion of this expression. The functional P_1 is not known. From this our considerations give us only some formal arguments to approximate the first term in expression (2.3) by a Boltzmann term. Nevertheless it can be seen that this term is an approximation for the case of 'small' deviations of the probability density function from an isotropic Gaussian.

Appendix B. Solution of the Fourier transformed PDE

The solution of the PDE (3.5) is done with the well known method of characteristics. The starting point is the characteristic system

$$\frac{\mathrm{d}k_1}{k_1} = \frac{\mathrm{d}k_2}{k_2} = \frac{\mathrm{d}k_3}{k_3 + Gk_1} = \frac{\mathrm{d}F}{\gamma F_0 - (Ga^{3j}_{1l}k_jk_l + \gamma)F}.$$

This ODE system is solved with k_1 as independent variable. The first three terms constitute two independent ODEs and consequently can be solved directly:

$$k_2 = C_2k_1, \tag{B 1}$$

$$k_3 = C_3k_1 + Gk_1 \ln k_1. \tag{B 2}$$

To avoid troublesome case differentiations use will be made of the symmetry $F(-\boldsymbol{k}) = F(\boldsymbol{k})$, therefore only $k_1 \geqslant 0$ is considered. The singularity in the characteristic system then is reached only from the right-hand side.

Insert k_2 and k_3 to solve the third equation of the characteristic system for $F(k_1)$,

$$\frac{\mathrm{d}F}{\mathrm{d}k_1} + \left(\frac{\gamma}{k_1} + a(k_1)\right) F = \frac{\gamma}{k_1} F_0(k_1, C_2k_1, C_3k_1 + Gk_1 \ \log k_1)$$

with

$$\begin{aligned} a(k_1, C_2, C_3) &= Ga^{3j}_{1l}\frac{k_jk_l}{k_1} \\ &= Gk_1 \left[a^{31}_{11} + (a^{32}_{11} + a^{31}_{12})C_2 + (a^{33}_{11} + a^{31}_{13})(C_3 + G\ln k_1) + a^{32}_{12}C_2^2 \right. \\ &\quad \left. +(a^{33}_{12} + a^{32}_{13})C_2(C_3 + G\ln k_1) + a^{33}_{13}(C_3 + G\ln k_1)(C_3 + G\ln k_1)\right]. \end{aligned} \tag{B 3}$$

As usual we seek first the homogeneous solution and then with the method of variation of constants a particular one

$$F = F_h + F_i \tag{B 4}$$

with

$$F_h = C_1 \ \exp\left(-\int_{k_h}^{k_1} \left(\frac{\gamma}{x} + a(x, C_2, C_3)\right) \mathrm{d}x\right) = C_1 \left(\frac{k_h}{k_1}\right)^{\gamma} \exp\left(-\int_{k_h}^{k_1} a(x, C_2, C_3)\mathrm{d}x\right); \tag{B 5}$$

$k_1 \to \infty$ yields the limit $F_h \to 0$, because in $a(k_1, C_2, C_3)$ the term $\sim a^{33}_{13}G^3k_1(\log|k_1|)^2$ dominates with $a^{33}_{13} = \left(-\frac{4}{11} + \frac{5}{11}c_2\right) R_{13} > 0$ for $c_2 < \frac{4}{5}$ (equations (2.8), (2.9)). This statement is independent of k_h, so we set $k_h = 1$ for the lower integration limit.

The particular solution reads

$$F_i(k_1, C_2, C_3) = \gamma \int_{k_u}^{k_1} \left(\frac{x}{k_1}\right)^{\gamma} \exp\left(\int_{k_1}^{x} a(x', C_2, C_3)\mathrm{d}x'\right) \frac{F_0(x, C_2x, C_3x + Gx\log x)}{x} \mathrm{d}x. \tag{B 6}$$

Choosing $k_u = 0$ one can derive the limit $\lim_{k_1\to 0} F_i(k_1, C_2, C_3) \to 1$ for all C_2, C_3 with l'Hospital's rule, by extracting a factor $1/k_1^{\gamma}$ from the integral.

With equations (B 1), (B 2) and (B 4) with (B 5) and (B 6) solved explicitly in the integration constants, one can represent the general solution of the PDE (3.5) as $\Psi\,(C_1, C_2, C_3) = 0$ or in explicit form

$$C_1 = g\,(C_2, C_3)$$

and therefore

$$F = g(C_2, C_3)\;\exp\left(-\int_{k_h}^{k_1}\left(\frac{\gamma}{x} + a(x, C_2, C_3)\right)\mathrm{d}x\right) + F_i\left(k_1, \frac{k_2}{k_1}, \frac{k_3}{k_1} - G\log k_1\right). \quad \text{(B 7)}$$

Now we show that the function g must vanish identically. For this we consider a path with $k_1, k_2, k_3 \to 0$ in the special manner that $C_2 = k_2/k_1$ and $C_3 = k_3/k_1 + G\ln k_1$ can take any ambiguous but constant value. We have seen already that in this case the normalization condition $F \to 1$ is fulfilled by F_i alone. Because the exponential function in the first term of equation (B 7) has non-zero values, it follows that $g(C_2, C_3) = 0$ for any C_2, C_3.

The solution of the PDE is therefore (B 6), where C_2, C_3 are replaced by the k_i. By introducing $\xi := x/k_1$ one can simplify

$$F(\boldsymbol{k}) = \gamma\int_0^1 \xi^{\gamma-1}\;\exp\left(\int_{k_1}^{\xi k_1} a(x', C_2, C_3)\mathrm{d}x'\right)$$
$$\times\exp\left(-\frac{\left[\frac{2}{3}E\right]}{2}\xi^2\left(k_1^2 + k_2^2 + (k_3 + k_1 G\log\xi)^2\right)\right)\mathrm{d}\xi.$$

Although this transformation is allowed only for $k_1 \neq 0$, this term yields the correct continuation for $k_1 = 0$. The main advantage of this transformation is that all the terms in the exponent can be represented as a quadratic form in $\boldsymbol{k}$:

$$\int_{k_1}^{\xi k_1} a\left(x', \frac{k_2}{k_1}, \frac{k_3}{k_1} - G\log k_1\right)\mathrm{d}x' = M_{ij}k_ik_j.$$

This calculation is cumbersome and was left to the computer algebra program 'Maple'. The result gives equation (3.6).

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