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**ANALYSE D'UN MODELE PDF DANS LE CAS D'UNE
COUCHE DE MELANGE**

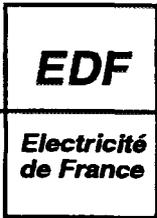
ANALYSIS OF A PDF MODEL IN A MIXING LAYER CASE

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MINIER J.P.
POZORSKI J.

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SYNTHÈSE :

L'objet de ce rapport est de présenter une analyse d'un modèle PDF (Probability Density Function) et une illustration des possibilités de cette approche sur le cas d'une couche de mélange.

La première partie présente les principes de l'approche PDF et l'utilisation de modèles stochastiques selon un point de vue Lagrangien. Le modèle retenu est celui de Pope (1991) et comprend des équations d'évolution sur les positions, vitesses et dissipations d'un grand nombre de particules.

Les développements sont validés en analysant les prédictions numériques par rapport aux mesures expérimentales sur le cas d'une couche de mélange. Cet exemple permet d'illustrer les capacités du modèle à prendre naturellement en compte l'intermittence interne et à correctement simuler l'intermittence externe. Une analyse physique basée sur la séparation des particules entre sous-classes laminaires et turbulentes est proposée pour justifier l'introduction dans le modèle de variables telles que l'énergie turbulente pondérée par la dissipation.

EXECUTIVE SUMMARY :

A recent turbulence model put forward by Pope (1991) in the context of PDF modelling has been applied to a mixing layer case. This model solves the one-point joint velocity-dissipation pdf equation by simulating the instantaneous behaviour of a large number of Lagrangian fluid particles. Closure of the evolution equations of these Lagrangian particles is based on diffusion stochastic processes.

The paper reports numerical results and tries to analyse the physical meaning of some variables, in particular the dissipation-weighted kinetic energy and its relation with external intermittency.

ANALYSIS OF A PDF MODEL IN A MIXING LAYER CASE

J.P. Minier¹ and J. Pozorski²

¹Laboratoire National d'Hydraulique, 6 Quai Watier 78400 CHATOU

²Institute of Fluid-Flow Machinery, Polish Academy of Sciences, Gdańsk, Poland

INTRODUCTION

Among the different approaches to the problem of turbulence modeling, the so-called PDF methods stand out as particularly attractive candidates. One of their main advantages is that they treat processes such as convection and source terms, however non-linear and complicated, in an exact way. The latter property is of major interest for situations involving chemical reactions and PDF methods have become popular for the simulation of combustion-related problems. Yet, since PDF methods completely model the one-point statistical behaviour in a flow and yields therefore far more information than classical moments closure, they are also very useful for other problems requiring a detailed description of turbulence. This is, for example, the case of Lagrangian two-phase flow models where the instantaneous fluid velocities encountered by particles along their trajectories are needed to simulate particle dispersion.

The model retained here is the one developed by Pope and coworkers (Haworth & Pope, 1986, 1987; Pope & Chen, 1990 and Pope, 1991). These papers are referred to for a detailed presentation and we limit ourselves to outlining the main aspects of the velocity and dissipation stochastic models. The aim of the present paper is twofold. It first reports results using Pope's model in a mixing case case which have been obtained with a numerical code developed independently. Validity is assessed by considering averaged variables up to third-order velocity moments. A second purpose is to investigate more specifically the ability of the model to reproduce characteristic features of turbulence such as deviation of velocity pdf from Gaussianity in regions of anisotropic turbulence and external intermittency. Results are used to shed some light on the physical signification of the variables which enter the model.

STOCHASTIC MODELLING

Pdf equation and Lagrangian model

As indicated by their name, PDF methods consist in modelling and solving the equation satisfied by the probability density function that the state variables have a given value. This equation is then solved by a Monte-Carlo method in which Lagrangian particles are introduced and regarded as representing samples of the pdf or independent realizations of the flow. In the following, we adopt a slightly different (yet equivalent) point of view in line with classical statistical reasoning. We immediately introduce the Lagrangian point of view and we consider a large number of fluid particles taken as small elements of fluid or points moving in a field. These particles interact through the pressure gradient and the viscous force. Just as in classical mechanics, the pdf equation is closed at the N -particle level and, in the limit $N \rightarrow +\infty$, it shows that the turbulence problem is closed at the characteristic functional level. We are interested in the first level of the hierarchy which corresponds here to the one-particle pdf $f(t, \mathbf{Y}_0)$ that the variables \mathbf{Y} attached to each particle take the value \mathbf{Y}_0 . The general pdf equation writes :

$$\frac{\partial f(t, \mathbf{Y})}{\partial t} = -\frac{\partial}{\partial Y_i}[\langle F_i | \mathbf{Y} \rangle f(t, \mathbf{Y})], \quad (1)$$

where $\langle F_i | \mathbf{Y} \rangle$ stands for the expected value of the component F_i of the 'force' (or rate of change of the variable Y_i) conditioned on the present state.

Modelling principles

Terms appearing in the above equation are closed when the 'force' can be expressed in terms of the variables that are followed and have to be modelled otherwise. The two key points of the approach are thus the choice of the independent variables Y_i that will be considered and, of course, the models for the unclosed terms. In Pope's model, the variables attached to the particles are its location, velocity and dissipation rate \mathbf{x} , \mathbf{U} , and ϵ , respectively. The introduction of the dissipation rate along particle trajectories (Pope & Chen, 1990) allows the turbulent timescale to be calculated from the model instead of being provided from an external source. It is also physically reasonable since ϵ is a small-scale quantity which defines internal intermittency. Furthermore, the slow part of the fluctuating pressure gradient which acts on the particles can be written as :

$$\frac{1}{\rho} p'(x) = \frac{1}{4\pi} \int \frac{1}{2|x-y|} (\varphi^2(y) - \frac{1}{\nu} \epsilon(y)) dy \quad (2)$$

where $\varphi = |\nabla \times \mathbf{u}|$ is the fluid vorticity norm and ν the viscosity. It is thus seen that the dissipation enters the pressure gradient force whose mean conditioned value has to be modelled. This, in turn, suggests that the introduction of the vorticity as an independent variable could be the next step in the model. The evolution equations of the modelled particles, disregarding the mean viscous and the gravity terms, can be written as :

$$d\mathbf{x}^* = \mathbf{U}^*(t) dt \quad (3)$$

$$dU_i^* = -\frac{1}{\rho} \frac{\partial \langle p \rangle}{\partial x_i} dt + dA_i^*(t) \quad (4)$$

$$d\epsilon^* = dA_i^*(t). \quad (5)$$

The first equation expresses that convection is treated exactly. In the particle equation of motion, the fluctuating part of the force has to be modelled whereas the evolution equation of the dissipation has to be modelled altogether since it only involves small-scale quantities. The unknown terms $A^*(t)$ are modelled as stochastic processes, more precisely on diffusion processes. Application of these processes is suggested by Kolmogorov hypotheses and physical reasoning. Indeed, the sample functions of a diffusion process A_t are continuous and can be expressed as solutions of stochastic differential equations (Arnold 1974):

$$dA_t = D(t, A_t)dt + \sqrt{B(t, A_t)}dW \quad (6)$$

where $D(t, A_t)$ and $B(t, A_t)$ are respectively the so-called drift and diffusion functions and where dW stands for the Wiener process (Gaussian white noise).

Stochastic model for velocity

The evolution equation for particle velocities writes :

$$dU_i^* = -\frac{1}{\rho} \frac{\partial \langle p \rangle}{\partial x_i} dt + D_i dt + \sqrt{C_0 \epsilon^*} dW_i. \quad (7)$$

The diffusion term is closed with reference to the Kolmogorov theory (1941) which yields that the second order Lagrangian structure function

$$D_{L(ij)}(\Delta t) = \langle [u_i(t + \Delta t) - u_i(t)][u_j(t + \Delta t) - u_j(t)] \rangle$$

in the inertial range is given by $\delta_{ij} C_0 \epsilon^* \Delta t$ (Monin & Yaglom, 1971) where the instantaneous dissipation rate ϵ^* is used according to the refined Kolmogorov hypothesis (1962). Because of the assumption of local isotropy of turbulent flows at Re sufficiently high, the diffusion term retains the isotropic form even for inhomogeneous cases, due to the use of isotropic Wiener process. The total drift term has been separated into the mean pressure gradient and a secondary term D_i which must meet the zero-mean condition, $\langle D_i \rangle = 0$. This ensures that the mean Navier-Stokes equation is respected and, in turn, that no spurious drifts exist. This term is closed by reference to second-order modelling taking into account internal intermittency and writes (Pope, 1991) :

$$D_i = -\left(\frac{1}{2} + \frac{3}{4}C_0\right)\langle \omega \rangle \frac{\bar{k}}{k} u_i^* + G_{ij}^a u_j^* - \frac{3}{4}C_0[\tilde{A}_{ij}^{-1}(\omega^* u_j^* - \langle \omega u_j \rangle) - \left(\frac{\bar{k}}{k}\right)A_{ij}^{-1}(\omega)u_j^*]. \quad (8)$$

In the latter relation, G_{ij}^a (where the subscript a stands for anisotropic) represents a second-order tensor which is function of the mean velocities and of the Reynolds stresses. The normalized Reynolds stress tensor A and the turbulent kinetic energy k are given by :

$$k = \frac{1}{2}\langle u_i u_i \rangle \quad \text{and} \quad A_{ij} = \langle u_i u_j \rangle / \left(\frac{2}{3}\langle k \rangle\right), \quad (9)$$

while \tilde{A} and \tilde{k} are dissipation-weighted means :

$$\tilde{k} = \frac{1}{2}\langle u_i u_i \epsilon \rangle / \langle \epsilon \rangle \quad \text{and} \quad \tilde{A}_{ij} = \langle u_i u_j \epsilon \rangle / \left(\frac{2}{3}\langle \epsilon \rangle \tilde{k}\right). \quad (10)$$

Stochastic model for dissipation

The evolution equation for turbulent energy dissipation rate is built upon the refined Kolmogorov hypothesis which states that $\epsilon^*(t)$ is a lognormally-distributed random variable. The equation is developed not in terms of the dissipation ϵ itself but rather in terms of the turbulence frequency (relaxation rate) ω which is defined by :

$$\omega(\mathbf{x}, t) = \epsilon(\mathbf{x}, t) / \tilde{k}(\mathbf{x}, t). \quad (11)$$

The complete version for the general case of inhomogeneous turbulence writes (Pope 1991):

$$\begin{aligned} d\omega^* = & -\omega^* \langle \omega \rangle dt \left\{ S_\omega + C_\chi \left[\ln \left(\frac{\omega^*}{\langle \omega \rangle} \right) - \left\langle \frac{\omega}{\langle \omega \rangle} \ln \left(\frac{\omega}{\langle \omega \rangle} \right) \right\rangle \right] \right\} \\ & + \langle \omega \rangle^2 h dt + \omega^* \sqrt{2C_\chi \langle \omega \rangle \sigma^2} dW. \end{aligned} \quad (12)$$

In this equation, σ^2 is the variance of $\ln(\omega/\langle \omega \rangle)$, C_χ is a constant. Next, h represents a drift term and models the mechanism through which entrained laminar particles ($\omega^* = 0$) become turbulent. The source term h is larger near the edges of a turbulent stream where the flow is highly intermittent and decreases near the centre of such flows where a fully turbulent state is approached. It is related to the intermittency factor γ which can be defined as the local proportion of turbulent particles by $h = C_{\omega 3}(1 - \gamma^{1/2})^2$. S_ω stands for the normalized decay rate of $\langle \omega \rangle$ and is modelled by reference to the standard equation of $\langle \epsilon \rangle$:

$$S_\omega = (C_{\epsilon 2} - 1) - (C_{\epsilon 1} - 1) \frac{P}{\langle \epsilon \rangle}, \quad (13)$$

where P is the turbulent kinetic energy production term.

The constants of the model are $C_{\epsilon 1} = 1.37$, $C_{\epsilon 2} = 1.9$, $C_{\omega 3} = 1$, $C_\chi = 1.6$, $\sigma^2 = 1$, $C_0 = 3.5$.

Resulting mean equations

The equations for the statistical moments show that the mean continuity and the Navier-Stokes equations are exact while the second-order (Reynolds stress) equation is :

$$\begin{aligned} \frac{\partial}{\partial t} \langle u_i u_j \rangle & + \langle U_k \rangle \frac{\partial}{\partial x_k} \langle u_i u_j \rangle + \frac{\partial}{\partial x_k} \langle u_i u_j u_k \rangle \\ & + \langle u_i u_k \rangle \frac{\partial \langle U_j \rangle}{\partial x_k} + \langle u_j u_k \rangle \frac{\partial \langle U_i \rangle}{\partial x_k} \\ & = \langle u_i D_j \rangle + \langle u_j D_i \rangle + C_0 \tilde{k}(\omega) \delta_{ij} \\ & = -(1 + \frac{3}{2} C_0) \frac{\langle \epsilon \rangle}{k} (\langle u_i u_j \rangle - \frac{2}{3} k \delta_{ij}) \\ & \quad + G_{it}^a \langle u_j u_i \rangle + G_{jt}^a \langle u_i u_i \rangle - \frac{2}{3} \langle \epsilon \rangle \delta_{ij} \end{aligned} \quad (14)$$

The equation for the mean $\langle \omega \rangle$ is :

$$\left\langle \frac{d\omega}{dt} \right\rangle = \frac{\partial \langle \omega \rangle}{\partial t} + \langle U_i \rangle \frac{\partial \langle \omega \rangle}{\partial x_i} + \frac{\partial}{\partial x_i} \langle u_i \omega \rangle = -\langle \omega \rangle^2 (S_\omega - h). \quad (15)$$

It is thus seen that the present model is directly equivalent to second-order modelling with the further advantage that triple moments are in a closed form and do not have to be modelled. When the anisotropic matrix G^a is put to zero as was done in the calculations, the model gives the Rotta return to isotropy term.

APPLICATION IN A MIXING LAYER

Numerical simulations have been performed in a mixing layer. The algorithm implemented is the boundary-layer algorithm (Pope, 1985) where particles represent a fixed amount of axial momentum instead of a fixed amount of mass and are marched downstream until a self-similar state is reached. Details of the numerics as well as of the results are presented elsewhere (Pozorski & Minier 1994). The number of particles varied from around 10,000 at the beginning to about 100,000 at the end. The mixing layer was simulated with the two free stream velocities $U_{low} = 1m/s$ and $U_{up} = 1.5m/s$ respectively. The computed spreading rate is 0.036 which compares well with experimental values which can be expressed by (Townsend, 1976) :

$$S \simeq 0.185 \frac{U_{up} - U_{low}}{U_{up} + U_{low}} \sim 0.037. \quad (16)$$

Figure 1 presents the four non-zero Reynolds stress components. Agreement with experimental results is satisfactory, especially for the shear stress $\langle uv \rangle$ (directly related to the spreading of the layer) and the streamwise component $\langle u^2 \rangle$. Higher-order moments have been computed such as triple correlations and skewness and flatness factors of the velocity components (Figures 2 and 3).

external intermittency

Turbulence models based on the frequency rate ϵ/k have already been put forward dating back to Kolmogorov but the definition used in the present model is made in terms of the dissipation-weighted kinetic energy. The introduction of \hat{k} can be justified by the taking into account of external intermittency. At a given point, the flow is regarded as being made up of a turbulent subclass (with internal intermittency) and a non-turbulent subclass (without dissipation). Application of Kolmogorov's hypothesis is possible only in the turbulent subclass. Therefore, if we consider the Lagrangian velocity structure function $D_L = \langle (\Delta_t U)^2 \rangle$, we can write :

$$D_L^t = C_0 \langle \epsilon \rangle_t dt \quad (17)$$

where the subscript indicates the turbulent subclass. Since the averaged dissipation and the dissipation in the turbulent subclass are related through the external intermittency coefficient by $\langle \epsilon \rangle = \gamma \langle \epsilon \rangle_t$, we have as expected :

$$D_L = \gamma D_L^t = C_0 \langle \epsilon \rangle dt. \quad (18)$$

The turbulent Lagrangian velocity structure function can also be expressed with the turbulent frequency which (in the turbulent subclass) is naturally defined by $\omega_t = \epsilon_t/k_t$:

$$D_L^t = C_0 \langle \omega \rangle_t k_t dt. \quad (19)$$

Then, the unconditional Lagrangian velocity structure function is given by :

$$D_L = \gamma D_L^t = C_0 \gamma \langle \omega \rangle_t k_t dt. \quad (20)$$

ω used in the model represents the unconditional frequency as indicated by the presence of the drift term h . Its mean value $\langle \omega \rangle$ is the value averaged over the two subclasses and we have $\langle \omega \rangle = \gamma \langle \omega \rangle_t$. The two expressions of D_L then show that

$$\langle \omega \rangle = \frac{\langle \epsilon \rangle}{k_t}. \quad (21)$$

The kinetic energy of the turbulent subclass k_t can be related to \bar{k} using Kolmogorov theory which states that velocity fluctuations representative of the large scales are independent of the dissipation which characterizes the small scales.

$$\bar{k} = \frac{\langle \mathbf{u}^2 \epsilon \rangle}{\langle \epsilon \rangle} = \frac{\langle \mathbf{u}^2 \epsilon \rangle_t}{\langle \epsilon \rangle_t} \sim \langle \mathbf{u}^2 \rangle_t = k_t, \quad (22)$$

and the definition of the frequency becomes :

$$\langle \omega \rangle = \frac{\langle \epsilon \rangle}{\bar{k}}. \quad (23)$$

Since \bar{k} is an averaged variable, this reasoning can be extended to instantaneous values and justifies the definition of ω in (11). To illustrate and support that discussion, the mean values of the frequency conditioned on several values of the streamwise velocity (Figure 4) have been computed. Results obtained in four different cells for the mixing-layer case are presented. In each cell, the two subclasses turbulent and laminar were isolated and conditional mean dissipation were calculated as a function of a given value of the instantaneous streamwise velocity $(u - \langle u \rangle) / \langle u^2 \rangle^{1/2}$. These results are very similar to the experimental ones (Kuznetsov & Sabel'nikov, 1992). In the cells near the center of the layer ($\eta = \pm 0.046$) where external intermittency is negligible, ω and u appear as nearly independent. This is only approximate since there is clearly a link in the model, for example through the term S_ω in the ω -equation and ω and u cannot be strictly speaking independent. But the dependence appears to be weak. On the contrary, in cells more on the outskirts of the layer and where external intermittency is appreciable, results are quite different. There is a marked dependence between ω and u , but mainly as a result of external intermittency. Indeed, in the turbulent subclass, we retrieve the same weak dependence as near the center of the layer. The next figure (Figure 5) presents different calculations the external intermittency coefficient γ . The first one corresponds to the expression proposed by Pope (1991), $\gamma = \langle \omega^{1/2} \rangle / \langle \omega \rangle^{1/2}$. The second one is a direct calculation made in each cell by separating directly the turbulent particles from the laminar ones. Distinction is based on the dissipation which when plotted reveals two subclasses. Such a treatment is easily carried out in cells away from the center, but becomes somehow arbitrary as one moves towards the center that is when $\gamma \rightarrow 1$, that is when the two subclasses tend to merge. On the same figure, the ratio k/\bar{k} is also plotted. Results agree with experimental data and indicate that k/\bar{k} could be regarded as an approximation of the external intermittency factor by considering that the kinetic energy in the laminar subclass is negligible.

One-point velocity pdfs have also been considered and are plotted in Figures 6 and 7. Results are in qualitative agreement with the experimental analysis of Champagne *et al.* (1976) and show that the model is able to reproduce deviations from the normal distribution which is an important factor in inhomogeneous situations.

CONCLUSION

Results obtained with a PDF method have been analysed in a mixing layer case. The model consists in a Lagrangian simulation of a large number of fluid particles and represents a Monte-Carlo solution of the joint velocity-dissipation pdf equation. Closure of the diffusion terms is based on Kolmogorov's hypotheses. The drift terms are closed with reference to second-order modelling and the model is thus equivalent to a RSM model with regard to mean quantities. However, since it models the instantaneous behaviour of fluid particles, it contains a higher level of physical information on turbulence. The introduction of the dissipation rate as an independent variable is believed to represent a clear improvement. The turbulent timescale can be computed from the model but it also allows internal intermittency to be taken into account through Kolmogorov refined hypothesis. Since the model simulates both laminar and turbulent particles, external intermittency which is a typical feature of free shear flows can be calculated. An analysis has been put forward to reveal the physical signification of dissipation-weighted variable such as \tilde{k} and their relation with the intermittent factor.

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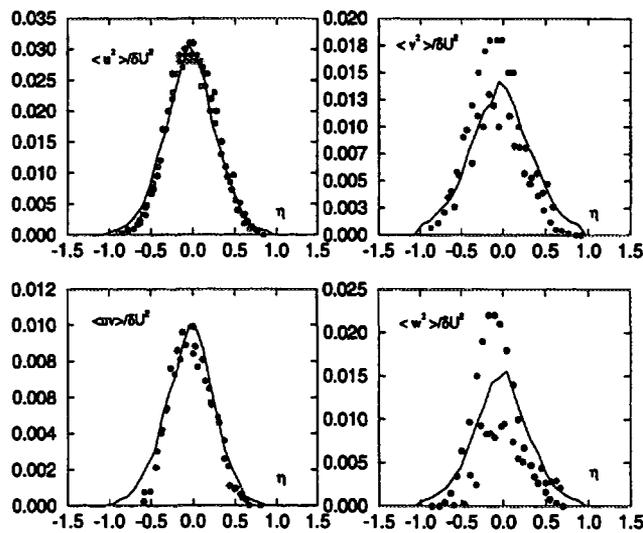


Figure 1: Reynolds stress components plotted as a function of the normalized cross-stream location $\eta = y/x/\delta$ where δ is the spreading rate. Comparison with the experiments of Wynanski & Fiedler (\bullet), Patel (\star) and Champagne *et al.* (\square).

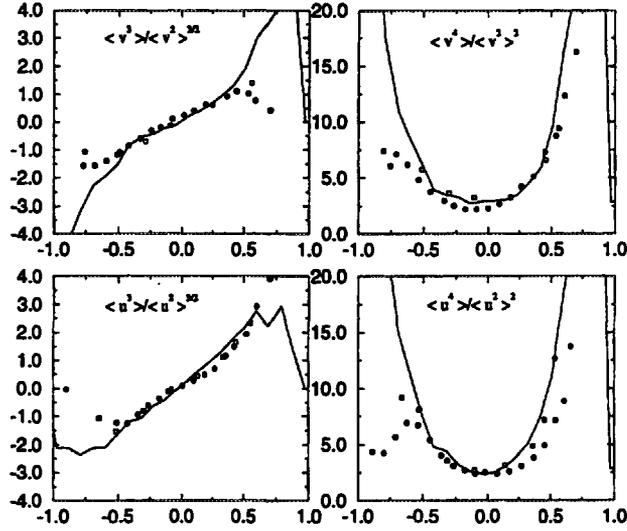


Figure 2: Skewness and flatness factors of the streamwise and the cross-stream velocity components. Comparison with the Wynanski & Fiedler (\bullet) and the Champagne *et al.* (\square) experiments.

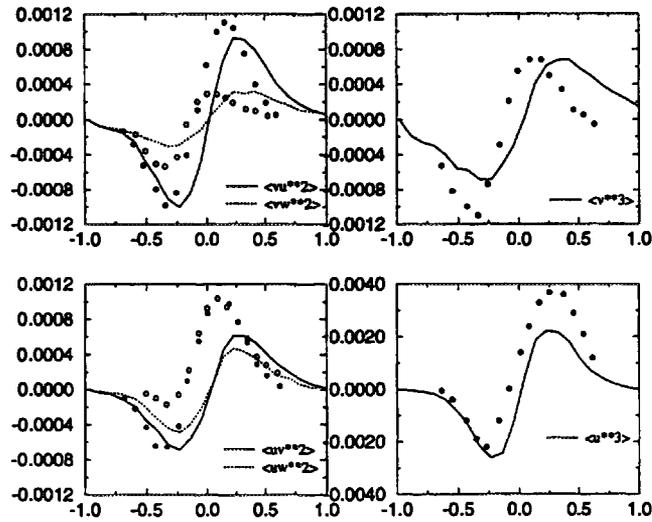


Figure 3: Various third-order velocity moments. Comparison with the Wynanski & Fiedler experiment. The solid line is to be compared with the closed symbol and the dotted line with the empty symbol.

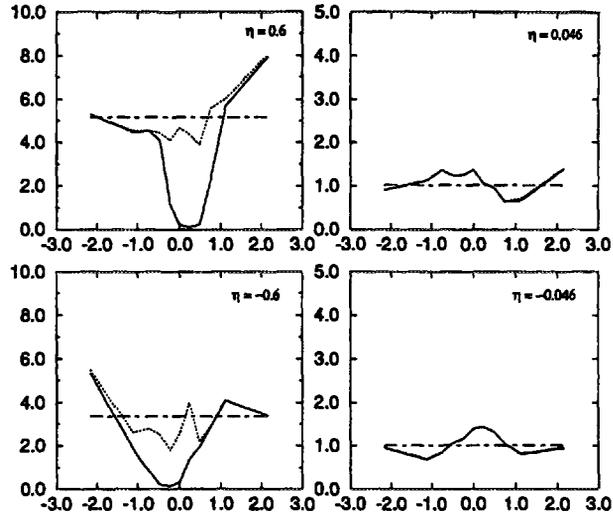


Figure 4: Calculation of the averaged dissipation at a given location. The solid represents the mean value of ω conditioned on a given value of the fluctuating streamwise velocity $\langle \omega | u \rangle / \langle \omega \rangle$. The dotted line represents the conditional mean of ω computed in the turbulent sub-class $\langle \omega_i | u \rangle / \langle \omega \rangle$. The dot-dashed line is the inverse of the external intermittency factor.

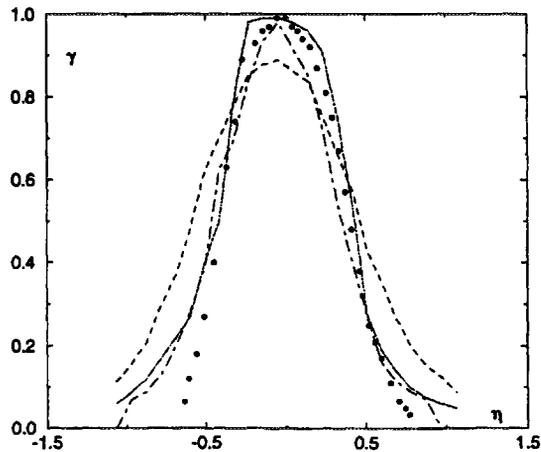


Figure 5: External intermittency coefficient. Comparison with the Wygnanski & Fiedler (●) experiment. The solid line represents a direct computation based on the fraction of turbulent particles in each cell. The dotted line is the evaluation of γ using the expression $(\omega^{1/2}) / \langle \omega \rangle^{1/2}$, while the dot-dashed one represents the ratio k / \bar{k} .

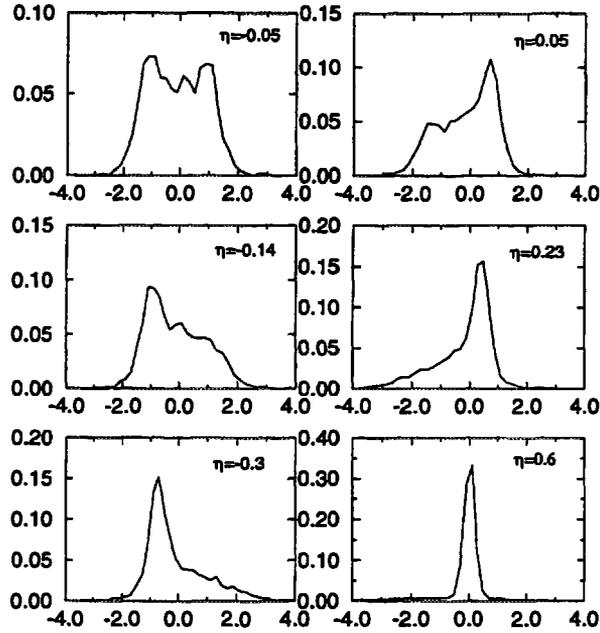


Figure 6: Histograms of the streamwise velocity component at different locations across the mixing layer. The distributions are centred and plotted as a function of the normalized value $(u - \langle u \rangle) / \langle u^2 \rangle^{1/2}$.

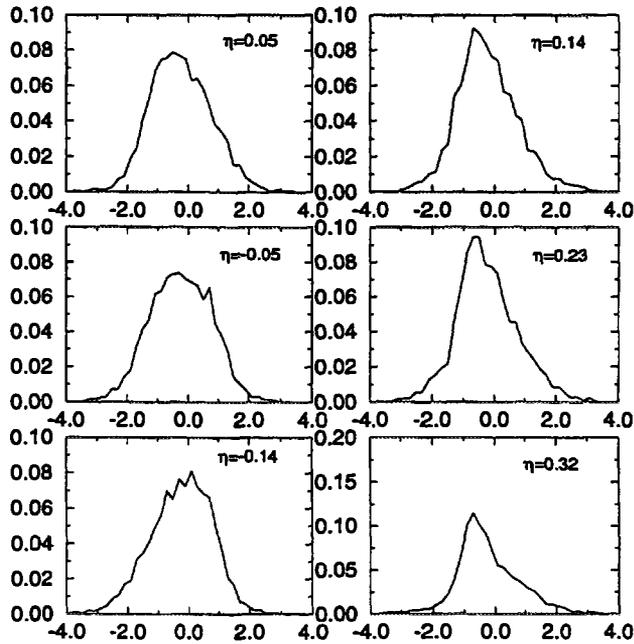


Figure 7: Histograms of the crosswise velocity component at different locations across the mixing layer. The distributions are centred and plotted as a function of the normalized value $(v - \langle v \rangle) / \langle v^2 \rangle^{1/2}$.