

**ON THE VALIDITY OF THE ASSUMED PDF  
METHOD FOR MODELING BINARY  
MIXING REACTION OF EVAPORATED VAPOR IN  
GAS/LIQUID-DROPLET TURBULENT SHEAR FLOW**

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## ABSTRACT

An investigation of the statistical description of binary mixing and/or reaction between a carrier gas and an evaporated vapor **species** in two-phase gas-liquid turbulent flows is performed through both theoretical analysis and comparisons with results from direct numerical simulations (**DNS**) of a two-phase mixing layer. **In** particular, the validity and added complications of extending single-point assumed probability density function (PDF) methods to two-phase flows involving evaporating droplets as sources of vapor are addressed. Noting that **Favre** density-weighted averaging is the most convenient form for moment transport equations for these flows, algebraic relationships are derived for the ratios of the **Favre** and non-weighted scalar *means* and variances. Comparisons with the **DNS results** indicates that the mixture fraction **Favre** moments are nearly identical to the corresponding non-weighted moments even at the mixing layer **centerline** where the rms density fluctuation is  $> 12\%$  of the mean density. It is therefore considered appropriate to use **Favre** moments for PDF closure. A transport equation for the **Favre** mixture fraction variance is then presented which contains four new terms **due** to evaporation effects. The **DNS results** indicate that one of these terms due to scalar-source correlations is predominantly responsible for scalar variance production, whereas the remaining three terms are of negligible magnitude. Finally, the  $\beta$  PDF which is known to represent well the **DNS generated mixture fraction** statistics for single-phase mixing, is shown to be a poor representation for mixing of vapor resulting from droplet evaporation.

## INTRODUCTION

Whereas probability density function (PDF) methods applied to binary mixing and reaction in single-phase turbulent flow have been investigated over the past two decades[1][2][3][4], the analogous two-phase problem involving a vapor species generated through liquid droplet evaporation remains **essentially** unaddressed. The simplest and most commonly used of the single-phase methods is the ‘assumed’ PDF method **which** is based on an *a priori* specification of an appropriate density for the mixture fraction. **Necessary**, but not sufficient, characteristics for a physically plausible assumed PDF *are* that it **be** bounded on a **finite domain** (i.e.  $0 \leq \phi \leq 1$ ) **and be** capable of accurately portraying the ‘true’ scalar density evolution throughout all stages of mixing; e.g. from initially segregated double delta **function** through asymptotically **fully** mixed Gaussian[5]. From **the perspective of implementation**, the two-parameter  $\beta$  PDF[4] is particularly attractive **due** to the simple algebraic relationships defining

its parameters in terms of the scalar mean and **variance**[4]. The  $\beta$  distribution **has** furthermore been shown to compare well with results obtained by direct numerical simulations (**DNS**) of a single-phase, non-homogenous reacting shear **layer**[6]. A procedure for generating PDFs appropriate for single-phase binary mixing was recently proposed by Miller et. **al.**[5] who introduced a family of PDFs based on the Johnson-Edgeworth Translation (JET). They evaluated one member of this family, the Logit-Normal PDF, along with the  $\beta$  and the Amplitude Mapping Closure (**AMC**)[7][8] through a comparison with DNS results of binary mixing in homogeneous isotropic turbulence. Although all of the PDFs captured the general features of the DNS scalar evolution, the **Logit-Normal** was found to most accurately portray the intermediate mixing stages; however, it is was not possible to obtain algebraic moment closures for this PDF and its practical application is therefore questionable. The present study addresses the question of the possible extension of the assumed PDF method to binary **mixing/reaction** occurring when one species is introduced through the evaporation of droplets in two-phase gas-liquid turbulent flows. This situation is different from the aforementioned studies because of additional complexities not found in single-phase flows.

Consider the transport equations for the gas phase density, evaporated vapor mass fraction and conserved scalar mixture fraction for this two-phase binary mixing problem:

$$\frac{\partial}{\partial t} (\rho) + \frac{\partial}{\partial x_j} [\rho u_j] = -S_V, \quad (1)$$

$$\frac{\partial}{\partial t} (\rho Y_V) + \frac{\partial}{\partial x_j} [\rho Y_V u_j] - \frac{\partial Y_V}{\partial x_j} = -S_V, \quad (2)$$

$$\frac{\partial}{\partial t} (\rho \phi) + \frac{\partial}{\partial x_j} [\rho \phi u_j] - \rho \Gamma \frac{\partial \phi}{\partial x_j} = 0, \quad (3)$$

where  $0 \leq \phi \equiv (1 + Y_c - Y_V)/2 \leq 1$  is the conserved scalar mixture fraction and  $S_V$  is a mass source/sink due to **vaporization/condensation** of the liquid phase ( $S_V$  is negative for evaporation). In this study it is assumed that the dispersed phase volume fraction is small, the species **diffusivity**  $\Gamma$  is constant and no reactions occur. However, for reacting flows **Eq.(3)** is unaltered, and the statistics of the reactants and products can be related **directly** to those of the mixture fraction (see e.g. **Ref.[6]**), so that the methodology presented here remains valid.

In general, the gas phase flow initially consists of a pure carrier species such that the scalar PDF is everywhere **unimodal** in the form of a delta **function** located at  $\phi = 1$  in mixture fraction space. As evaporation and mixing progress, the scalar distribution **will** grow inwards ( $\bar{\phi} < 1$ ; see the Nomenclature for averaging definitions) indicating a **more** mixed state which will be intuitively characterized by a highly skewed distribution **function**. The actual form of such a PDF will be determined by the coupled physical **evaporation/condensation and** turbulent mixing processes occurring within the flow and may vary substantially from that observed in single-phase binary mixing.

The present investigation addresses three issues associated with the statistical description of such two-phase flows by assumed PDF methods: (1) If there exists an appropriate PDF capable of portraying the mixture fraction evolution through all stages of mixing, then the non-weighted mean and variance are two moments necessary to determine the PDF. However, since the governing transport equations for the scalar moments are most conveniently cast in the form of **Favre** density-weighted averaging, we first **analyze** the conditions under which it is valid to substitute **Favre** moments for non-weighted moments for PDF determination. (2) **Favre** averaged transport equations for the mixture fraction mean and variance **are** then derived and the relative magnitudes of terms resulting from the evaporative source *S<sub>vare</sub>* calculated for the simulated shear flow. If an appropriate PDF exists, and if the **Favre** moments can be substituted for **the** non-weighted moments, then the solutions of these modeled equations **would** eventually be used to determine the assumed two-parameter PDF in **mixing/reaction** applications. (3) **The** assumed  $\beta$  PDF is tested with the **gas/liquid-droplet** mixing layer in order to characterize its applicability for two-phase evaporating droplet flow. The  $\beta$  PDF is chosen due to its relatively wide spread usage for single-phase **mixing/reaction** and to its algebraic closed form moment relations. The study is conducted through both theoretical analysis and through comparisons with results obtained previously from DNS.

## SIMULATION SUMMARY

Throughout the following analysis, previous DNS **results[9]** are used in conjunction with theoretical derivations;

the DNS results were for a shear layer formed by the merging of a pure gas stream with a hydrocarbon droplet laden gas stream. Since it is impossible to fully describe here the DNS results, only a brief summary of the simulation is included and the reader is referred to **Ref.[9]** for **further** details. The flow configuration considered is that of a three dimensional temporally developing mixing layer formed by the merging of two parallel flowing gas streams. The streamwise, cross stream and **spanwise** coordinate directions are denoted as  $x_1, x_2, x_3$ , respectively (i.e.  $u_1 = \pm U_0$  in the **far** fields of  $\pm x_2$ ). Periodic boundary conditions are employed in both the **streamwise** and spanwise directions, whereas adiabatic slip wall conditions are employed at the cross stream boundaries through the solution of appropriate characteristic **equations**[ 10]. Forcing of **fundamental** and first harmonic modes is used to stimulate **the** growth and development of both spanwise and **streamwise** disturbances resulting in a single primary vortex pairing. **The upper/unladen** stream ( $z_2 > 0$ ) is a pure gas phase flow (air), whereas the **lower/laden** stream is uniformly seeded with randomly placed spherical droplets with a liquid to gas mass loading of 0.225. Every individual droplet is tracked in a **Lagrangian** manner through the solution of equations for position, velocity, uniform internal temperature (infinite liquid thermal conductivity) and mass. Vaporization is governed by the **non-equilibrium** Langmuir-Knudsen evaporation **law**[11]. **All** properties are assumed to be constants, except for the latent heat of evaporation of the droplet species which is a **linear function** of temperature as required for calorically perfect **species**[9]. **The** gas phase viscosity is assumed to **be** independent of the mixture fraction, and is chosen to produce a resolvable flow ( $Re = 200$  based on the initial **vorticity** thickness and mean velocity difference across the layer), the **Prandtl** number is 0.697 and the Lewis number is assumed equal to unity. **All** remaining properties are calculated from correlations in Ref. [ 11 ] evaluated at **350K**, and correspond to those of air and **decane** for the carrier gas and liquid/vapor species, respectively. Complete two-way mass, momentum and energy exchange between phases is accounted for. The gas phase is initially at a uniform temperature of **350K** corresponding to moderate **evaporation** rates, the initial liquid phase temperature is **325K**, and the free stream Mach number is initially 0.5.

The DNS code utilizes fourth order accurate **Runge-Kutta** explicit time stepping for both **the** gas and droplet

equations, whereas **all** spatial derivatives are approximated by eight order accurate central finite differences [2]. The computational grid is analytically compressed in the cross stream direction with a maximal compression ratio of 0.5 at the centerline. Eulerian gas phase variables required for the dispersed phase transport equations are interpolated to the droplet positions using a fourth order accurate Lagrange interpolation procedure. Phase coupling terms (e.g.  $S_V$ ) are calculated by summing individual droplet contributions within local computational volumes using a geometric weighting factor based on the distance between each droplet and its eight nearest neighbor grid points. The solution procedure consists of integrating the coupled gas and droplet equations simultaneously in a time accurate manner following the **rollup** and spanwise vortex pairing of the mixing layer. **The** particular simulation addressed in this paper was performed with a gas phase resolution of 96 x 128 x 64 grid points, following  $4.5 \times 10^5$  individual droplets and required approximately 15 hours of CPU time on a Cray **J90 supercomputer**.

Figure 1 shows the final time mixture fraction PDF extracted from the DNS results as a **function** of the cross stream direction  $x_2$  (not the joint PDF). At this stage, the laden stream has reached a saturated state for which evaporation has essentially ceased (although droplets remain present) with  $\bar{\phi} \approx 0.94$  (i.e.  $\bar{Y}_V \approx 0.06$ ). In this case, saturation has occurred due to two primary influences: (1) evaporation and associated latent heat effects have reduced the temperature of the laden stream, and (2) the evaporated mass has resulted in a free stream vapor mass fraction approximately equal to the average surface mass fraction of the droplets. At this time the **saturated-free-stream** droplets have undergone an average **20%** reduction in mass; however, droplets which continue to be entrained into the layer undergo **further evaporation** as they are brought into contact with the higher temperature pure carrier gas stream. Inside the layer, a more markedly mixed state is apparent as characterized by a continuous range of mixture **fraction** values;  $0.92 < \phi \leq 1$ . Finally, the delta function located at  $\phi = 1$  for  $X_2 > 0$  locations indicates the pure carrier gas stream. The **successful** application of the assumed PDF method to this flow requires the accurate reproduction of the scalar distributions in Fig. 1 for all cross stream locations by an appropriate *a priori* chosen PDF.

## RESULTS

The presence of evaporative source terms in the gas phase density equation [Eq.(1)] implies that appropriate moment transport equations are most conveniently formulated in terms of **Favre** averaged (density-weighted) variables; even in the case of low speed flow. This is due to the fact that the **Favre** averaging removes terms resulting from density fluctuations **and** therefore substantially reduces the number of terms requiring modeling. In this section we investigate whether it is appropriate to determine an assumed PDF using **Favre** moments in **place** of the ‘true’ non-weighted averaged (hereinafter referred to as ‘ensemble’ averaged for simplicity) moments. Utilizing the standard definitions of the ensemble and **Favre** averaging **operators** defined in the Nomenclature, algebraic relationships between the corresponding means and variances of the scalar (or any flow variable) are derived:

$$\frac{\phi}{\bar{\phi}} = 1 + C_2(\rho, \phi) I(\rho) I(\phi), \quad (4)$$

$$\frac{\widetilde{\phi''\phi''}}{\phi''\phi''} = 1 - [C_2(\rho, \phi) I(\rho)]^2 + C_3(\rho, \phi, \phi) I(\rho), \quad (5)$$

where the correlation coefficient of order N:

$$C_N(a_1, a_2, \dots, a_N) = \frac{\overline{\prod_{k=1}^N a'_k}}{\prod_{k=1}^N (\overline{a_k'^2})^{1/2}}, \quad (6)$$

is bounded by  $-1 \leq C_N \leq +1$ , and the fluctuation intensity is defined as the root mean square (**rms**) fluctuation relative to the mean:

$$I(a_k) = (\overline{a_k'^2})^{1/2} / \bar{a}_k, \quad (7)$$

for any stochastic vector  $a_k$ . In this form, the above derivations clearly illustrate the physical constraints which must be satisfied in order to substitute **Favre** moments for ensemble moments. In particular, these relations suggest that moments calculated from the two methods may be nearly equal even in the case of large density fluctuations **if** either the scalar intensity is small or, more general] y, if the scalar and density fields are **uncorrelated** at order two and/or three.

The respective ratios of means and variances from Eqs.(4) and (5) are calculated from the final **time**’DNS results and presented in Fig. 2 along with the corresponding density values and correlation coefficients (averaging

is over homogeneous  $x_1 - x_3$  planes). These results show clearly that even for the present flow with relatively large density fluctuations [ $I(\rho)_{\max} > 0.12$ ; scc **Fig.2b**] that the **Favre** and ensemble means and variances are nearly identical. This is true for the means even in regions where the second order correlation coefficient is  $C_2(\rho, \phi) \approx -0.5$  (**Fig.2c**), because the scalar intensity is in all locations  $< 3\%$  (**Fig.2a**). The **Favre** and ensemble variances are also essentially identical, but for different reasons [note that the scalar intensity does not appear in **Eq.(5)**]: although **all** terms on the right hand side of **Eq.(5)** have maximal magnitudes within the layer, the respective terms due to second and third order correlations have opposite sign and cancel each *other* resulting in  $\widetilde{\phi''\phi''} \approx \phi''\phi''$ . **These results** suggest that it is reasonable to determine the assumed PDF with **Favre** moments for this flow **configuration**, and possibly for other flow types containing relatively large evaporation induced density fluctuations.

Determination of a two-parameter assumed PDF requires the knowledge of at least two moments of the scalar field. In general, closure is obtained through the solution of appropriate transport equations for the two lowest moments; i.e. the scalar mean and **variance**[5]. The **Favre** and ensemble averaging operators are therefore applied to **Eq.(3)** in order to obtain a transport equation for the **Favre** mean mixture fraction:

$$\frac{\partial}{\partial t} (\bar{\rho}\tilde{\phi}) = -\frac{\partial}{\partial x_j} [\bar{\rho}\tilde{\phi}\tilde{u}_j] + \frac{\partial}{\partial x_j} \left[ \bar{\rho} \Gamma \frac{\partial \tilde{\phi}}{\partial x_j} \right] - \frac{\partial}{\partial x_j} [\bar{\rho}\tilde{\phi}''u_j''], \quad (8)$$

and also, by invoking the continuity equation, for the **Favre** scalar variance evolution:

$$\frac{\partial}{\partial t} (\bar{\rho}\tilde{\phi}''\phi'') = I + II + III + IV + V + VI + VII + VIII + IX, \quad (9)$$

where the right hand side terms are given by:

$$I = -\frac{\partial}{\partial x_j} \left[ \bar{\rho} (\tilde{\phi}''\phi'') \tilde{u}_j \right] : \quad \text{Convection}, \quad (10)$$

$$II = +\frac{\partial}{\partial x_j} \left[ \bar{\rho}\Gamma \frac{\partial}{\partial x_j} (\tilde{\phi}''\phi'') \right] : \quad \text{Diffusion}, \quad (11)$$

$$III = -\frac{\partial}{\partial x_j} \left[ \bar{\rho} (\phi''\phi''u_j'') \right] : \quad \text{Third Order Turbulent Transport}, \quad (12)$$

$$IV = -2\bar{\rho} (\phi''u_j'') \frac{\partial \tilde{\phi}}{\partial x_j} : \quad \text{Mean Gradient Production}, \quad (13)$$



$$V = -2 \bar{\rho} \Gamma \left( \frac{\partial \widetilde{\phi''} \partial \phi''}{\partial x_{i,j} \partial x_{i,j}} \right); \quad \text{Dissipation,} \quad (14)$$

$$VI = + \overline{\phi'' \phi''} \overline{S_V}; \quad \text{Mean Source Destruction,} \quad (15)$$

$$VII = + 2 \tilde{\phi} \overline{\phi''} \overline{S_V}; \quad \text{Ensemble Mean of Favre Scalar Fluctuation Effect,} \quad (16)$$

$$VIII = + 2 \tilde{\phi} \overline{\phi'' S_V'}; \quad \text{Second Order Scalar-Source Correlation,} \quad (17)$$

$$IX = + \overline{\phi'' \phi'' S_V'}; \quad \text{Third Order Scalar-Source Correlation.} \quad (18)$$

Due to conserved nature of  $\phi$ , **Eq.(8)** is unaltered from its traditional single-phase form by **the** presence of droplets, and therefore will **not** be addressed in this paper. In contrast, the scalar variance equation contains, in addition to the traditional single-phase sources, four separate terms (**VI – IX**) which result from droplet evaporation. Note that these terms combine ensemble and **Favre** averaging of the scalar field due to the source term in **Eq.(1)** not containing the gas phase density. Terms **VI** and **VII** both *involve the* ensemble mean source term: the first of these is a destruction term for a vaporizing liquid phase as  $S_V$  takes negative values for evaporation, whereas the second term (**VII**) is proportional to the ensemble mean of the **Favre** scalar fluctuation (it is straightforward to show that  $\overline{\phi''} = \bar{\phi} - \tilde{\phi}$ ) which can be expected to become small under the conditions of **Eq.(4)**. Finally, terms **VIII** and **IX** involve second and third order scalar-source correlations, respectively. It is not readily apparent whether these last two terms will act as sources or sinks in general turbulent flows; however, physical intuition dictates that evaporating droplets should enhance the **scalar** variance. Since term **VI** is negative definite for evaporation and term **VII** should be small due to  $\overline{\phi''}$ , it may be conjectured that either the second and/or **the** third order scalar-source correlation must be a primary production term.

Figure 3 depicts the normalized magnitudes of the terms on the right hand side of the scalar variance transport equation calculated from the DNS results for three different times. In **all** cases, the scalar variance production near the center of the layer is primarily due to **the** action of both the mean gradient production (term **IV**) and the second order scalar-source correlation (term **VIII**). For this particular flow, all remaining terms due to **liquid** evaporation are of negligible magnitude during all stages of the mixing layer growth. It is interesting to note that

knowledge of the mean evaporation rate  $\overline{S_V}$  is of *no* direct use in solving the scalar variance equation since the two terms involving  $\overline{S_V}$  are both of negligible magnitude. Efforts directed at modeling the influence of evaporation on the scalar variance transport will therefore primarily require models for the correlation  $\overline{\phi'' S_V'}$ .

Assuming an accurate prediction of the scalar moments, the issue of whether or not the assumed PDFs generally applied to single-phase flow can be extended to the two-phase mixing layer is now addressed. Due to its available algebraic moment expressions, we test the utilization of the  $\beta$  PDF as specified by the scalar **Favre** mean and variance (calculated here from the DNS results) by comparing it with the DNS results. The  $\beta$  PDF will be deemed usable if it captures the various forms of the ‘true’ scalar PDF shown in Fig. 1 for all cross stream **locations**. Although in general the two parameters specifying the  $\beta$  PDF will be calculated from the solutions of the modeled **Eqs.(8)** and (9), in this case the two parameters are calculated from the ‘exact’ **Favre** mean and variance extracted from the DNS results. Figure 4 presents a comparison of the normalized third (skewness,  $\mu_3$ ) and fourth (flatness,  $\mu_4$ ) moments extracted from the DNS results as compared to the corresponding assumed PDF predictions. In the droplet laden stream ( $z_2 < 0$ ) the  $\beta$  density predicts an approximate Gaussian PDF (i.e.  $\mu_3 = 0$  and  $\mu_4 = 3$ ), whereas the DNS results show a much narrower distribution about the mean with  $\mu_4 \approx 2$ . Inside the layer, the assumed PDF is incapable of capturing the hump observed for both moments **located** near  $x_2/\delta_\omega \approx -0.8$  which results from the action of the vortex pairing engulfing fluid from the opposite pure gas stream into the layer. Within the  $x_2 > 0$  portion of the layer, both the skewness and flatness are over-predicted in magnitude, although the general profiles of the DNS moment curves are reproduced. Figure 5 more closely illustrates the problems with the assumed density by depicting both the DNS and  $\beta$  PDF predictions at the centerline,  $x_2 = 0$ . The  $\beta$  PDF is incapable of capturing the highly skewed and double hump features of the DNS scalar field (note that **the**  $\beta$  PDF is defined continuously over the range  $0 \leq \phi \leq 1$ ). **Finally, note that these results** represent a relatively strenuous test of the assumed PDF method, as the DNS PDFs are highly skewed due to the observed flow saturation. Further tests are recommended at higher temperatures for which the scalar mean will be decreased and the resulting PDF less severely skewed.

## CONCLUSIONS

The results described above have addressed several issues involved in **the** stochastic modeling of binary mixing **and/or** reaction in two-phase turbulent flows by assumed PDF methods. The mixing **and/or reaction** occurs between a carrier gas and a vapor resulting from liquid droplet evaporation. We first noted that PDF determination is most simply obtained through transport equations formulated in terms of **Favre** density-weighted moments due to the relatively **large** density fluctuations which result from evaporation effects. Accordingly, we have made the following three **contributions**: (1) We have derived algebraic relations which illustrate the conditions under which PDF determination can be accurately performed using **Favre** moments. We confirmed, using previously obtained DNS results, that **this** assumption is indeed valid for the two-phase mixing layer under conditions of moderate evaporation. (2) We have derived transport equations for the mixture fraction **Favre** mean and **variance**, and used the DNS results to calculate the relative *importance* of the four terms involving evaporation effects. We found that one term due to scalar-source correlations is responsible for variance production, whereas the remaining terms are of negligible magnitude. (3) We used the DNS results to illustrate inadequacies inherent in assuming the  $\beta$  PDF to portray the mixture fraction PDF evolution in two-phase mixing layers involving a dispersed liquid droplet species. Since this result was found for moderate evaporation, it is expected that this will represent a worst case situation since the resulting DNS mixture fraction PDFs are highly skewed. Future research in this area should focus on the derivation of new **PDFs** capable of capturing the unique characteristics of the two-phase mixture fraction statistics.

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## NOMENCLATURE

- $a_k$  Generic stochastic vector.
- $C_N$  Correlation **coefficient** of order  $N$ .
- $I$  Normalized fluctuation intensity.
- $Re$  Reynolds number.
- $S_V$  Source term due to liquid **evaporation/condensation (negative/positive)**.
- $t$  Time.
- $u_i$  Velocity vector.
- $U_0$  Mean free stream velocity ( $A U_0 = 2U_0$ ).
- $Y_C$  Carrier gas mass fraction.
- $Y_V$  Vapor evaporate mass **fraction**.
- $\delta_\omega$  **Vorticity** thickness =  $\Delta U_0 / (d\bar{u}_1/dx_2)_{\max}$ .
- $\delta_{\omega,0}$  Vorticity thickness at  $t = 0$ .
- $\Gamma$  **Fickian diffusion** coefficient.
- $\rho$  Gas **phase** density.
- $\phi$  Mixture fraction scalar variable ( $0 \leq \phi \leq 1$ ).
- $\mu_N$  **Normalized** moment of order  $N$ :  $\mu_N(a_k) = \overline{(a'_k)^N} / \overline{(a'_k)^2}^{N/2}$
- $\bar{a}_k$  Non-weighted ensemble average of  $a_k$ .
- $\widetilde{a}_k$  Density-weighted **Favre** average of  $a_k$ :  $\widetilde{a}_k = \overline{\rho a_k} / \bar{\rho}$ .
- $a'_k$  Fluctuation of  $a_k$  with respect to  $\bar{a}_k$ .
- $a''_k$  Fluctuation of  $a_k$  with respect to  $\widetilde{a}_k$ .

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## FIGURE CAPTIONS

Figure 1: Instantaneous mixture fraction PDF extracted from the **DNS** results as a function of the cross stream direction at time  $t\Delta U_0/\delta_{\omega,0} = 50$ .

Figure 2: Pertinent flow statistics across the layer at DNS time  $t\Delta U_0/\delta_{\omega,0} = 50$ : (a) Comparison of the ensemble and **Favre** scalar mean and rms, (b) Ensemble mean and rms density, (c) Second and third order density-scalar correlation **coefficients**.

Figure 3: Normalized source terms from the **Favre** variance transport equation as a function of the cross stream direction at times (a)  $t\Delta U_0/\delta_{\omega,0} = 10$ , (b)  $t\Delta U_0/\delta_{\omega,0} = 25$ , (c)  $t\Delta U_0/\delta_{\omega,0} = 50$ .

Figure 4: Comparison of skewness ( $\mu_3$ ) and flatness ( $\mu_4$ ) calculated from DNS results (at time  $t\Delta U_0/\delta_{\omega,0} = 50$ ) with predictions based on an assumed  $\beta$  PDF.

Figure 5: Comparison of the scalar PDF extracted from the DNS results at  $t\Delta U_0/\delta_{\omega,0} = 50$  and  $X_2 = 0$  with the assumed  $\beta$  PDF prediction.

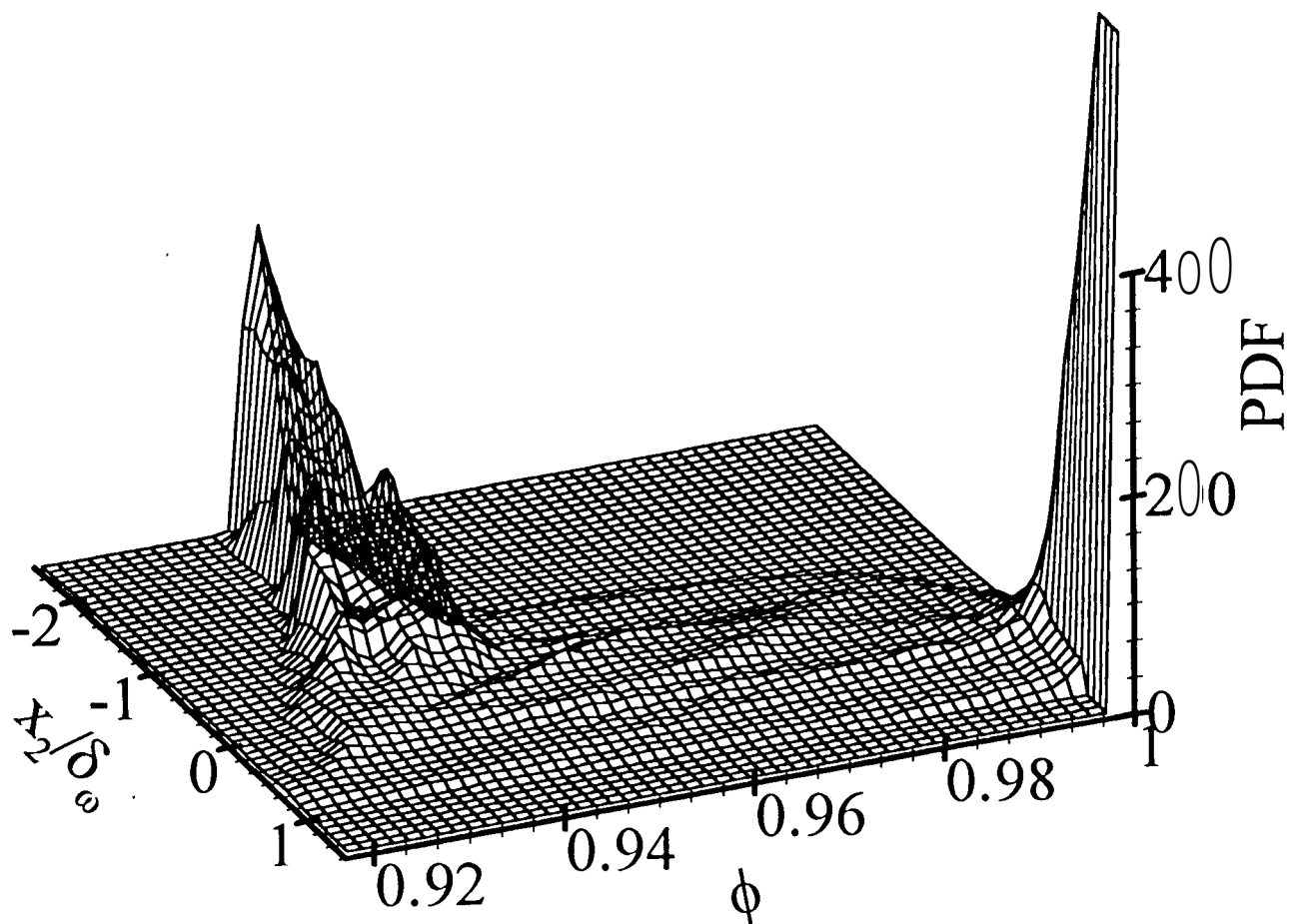


Figure 1

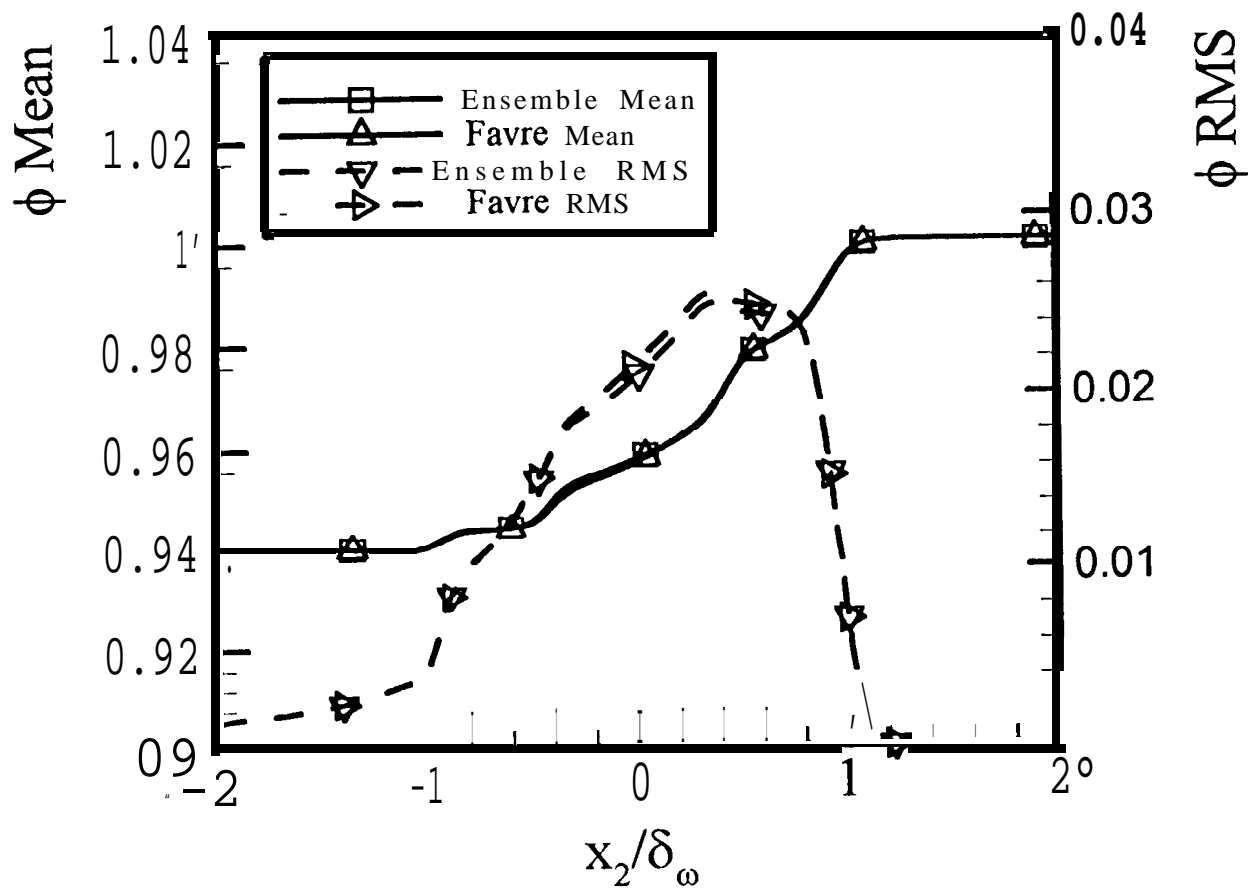


Figure 2a



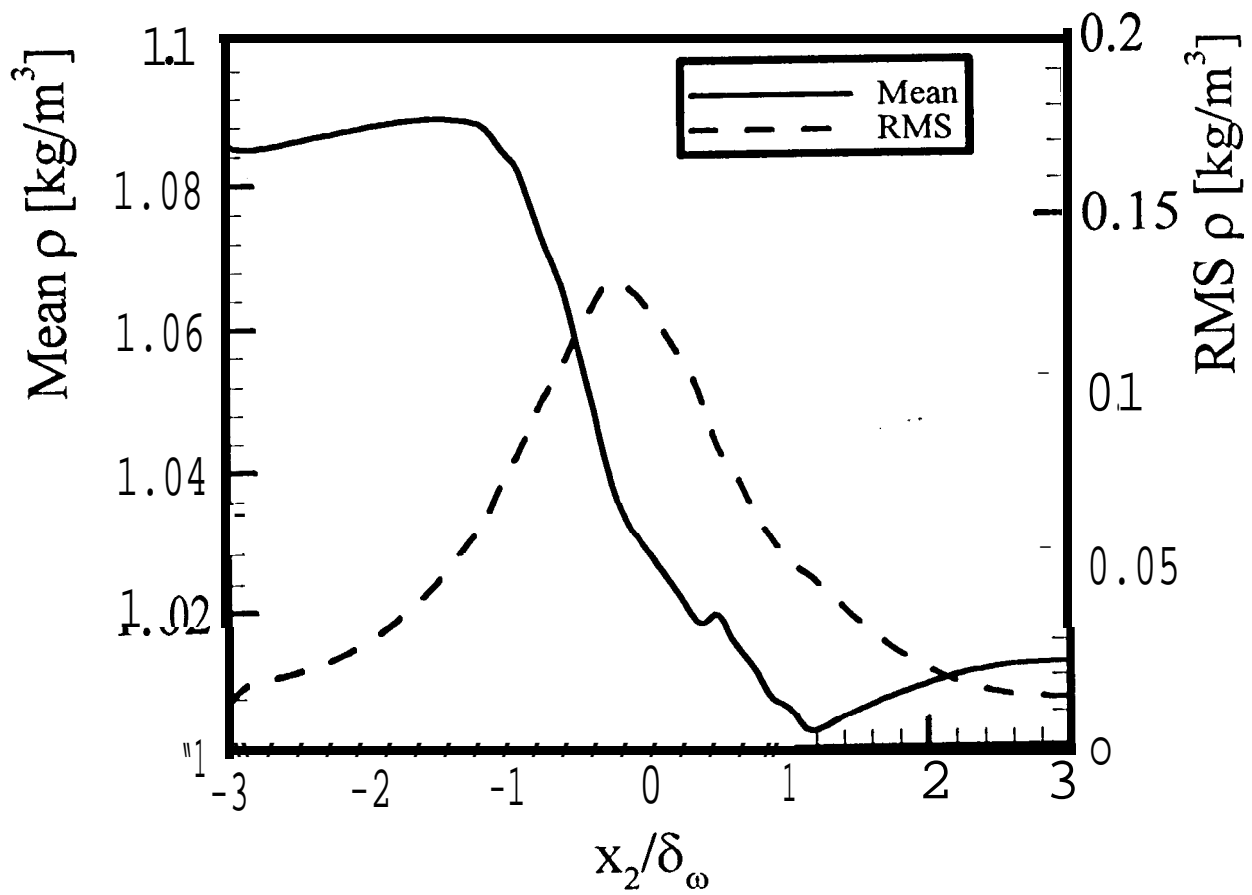


Figure 2b

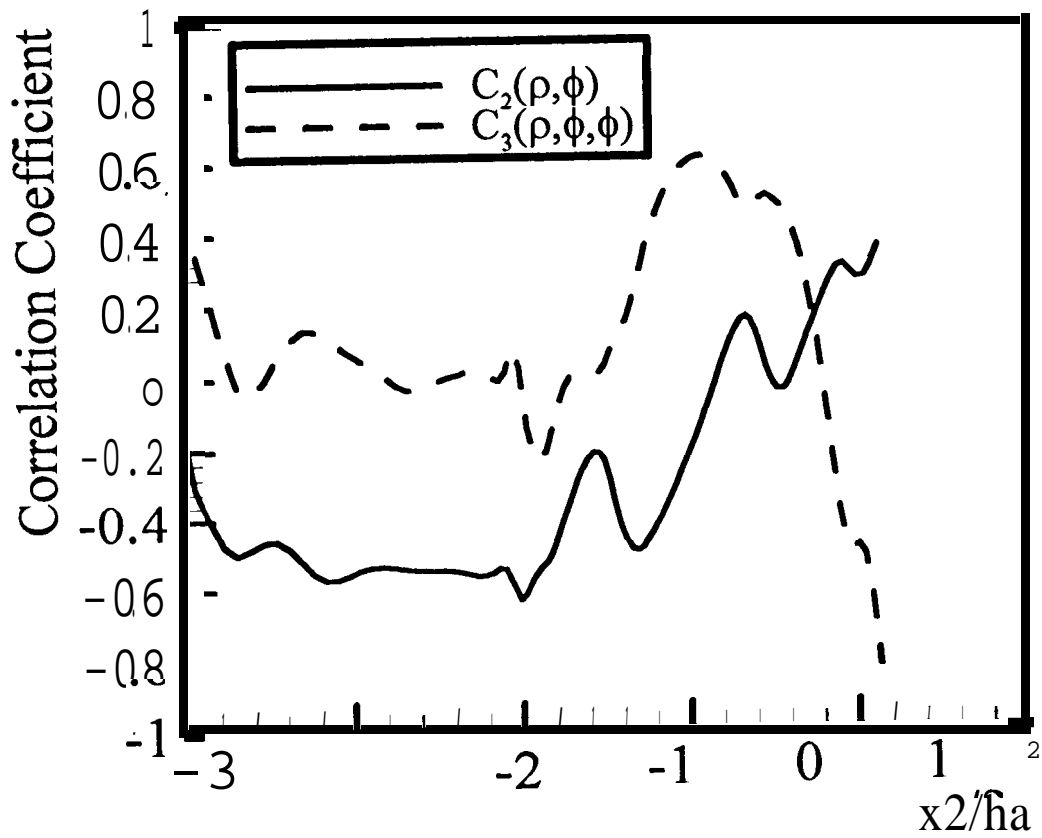


Figure 2 c

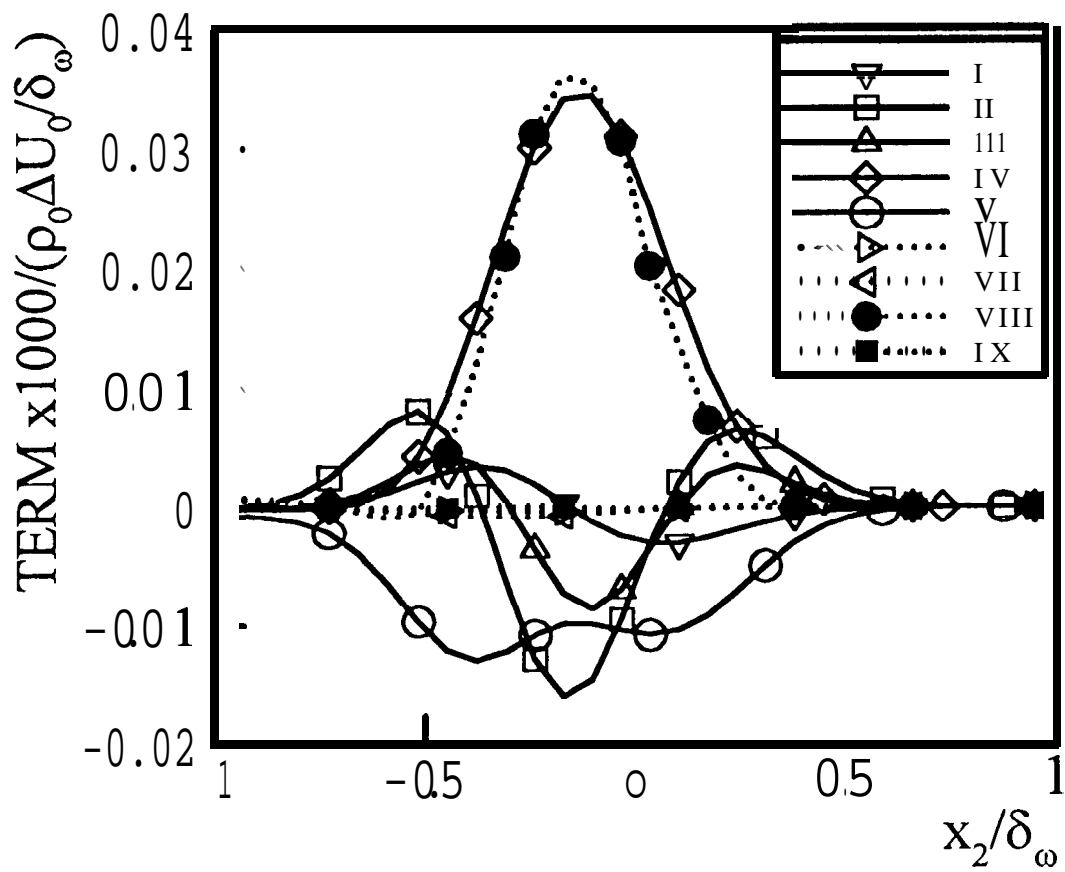


Figure 3a

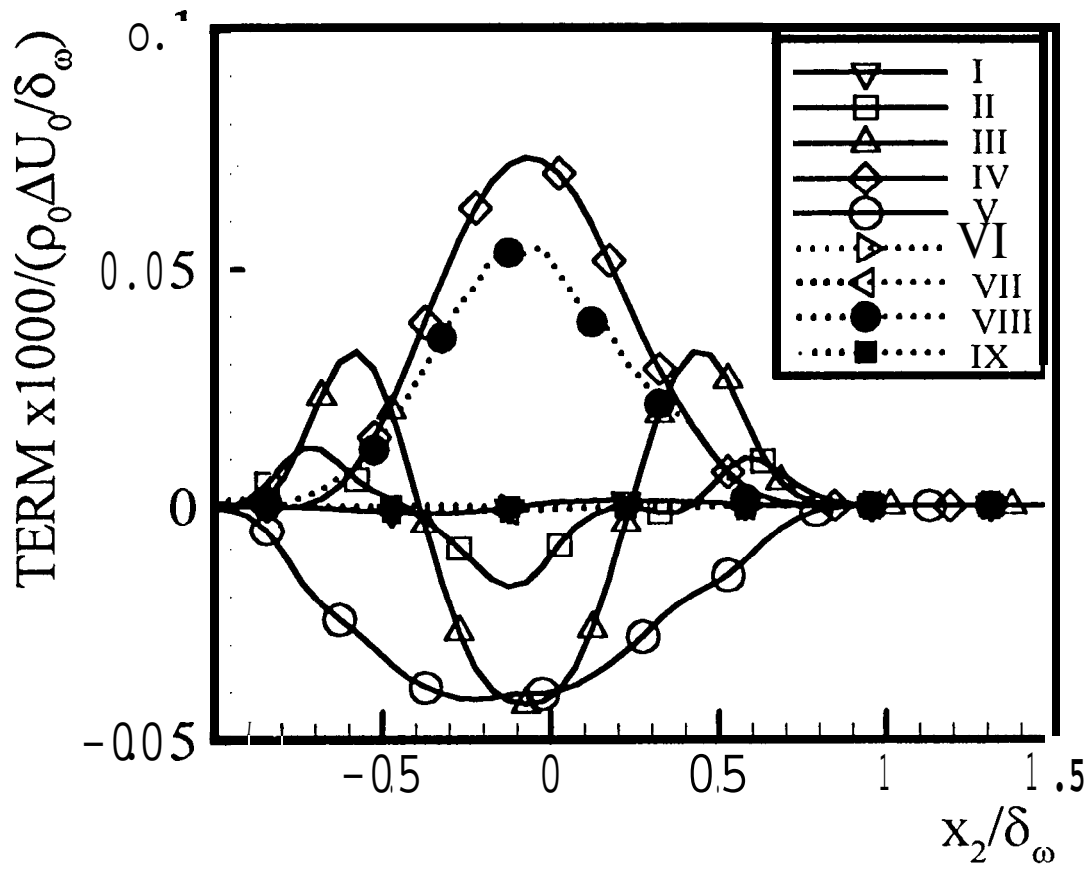


Figure 3b

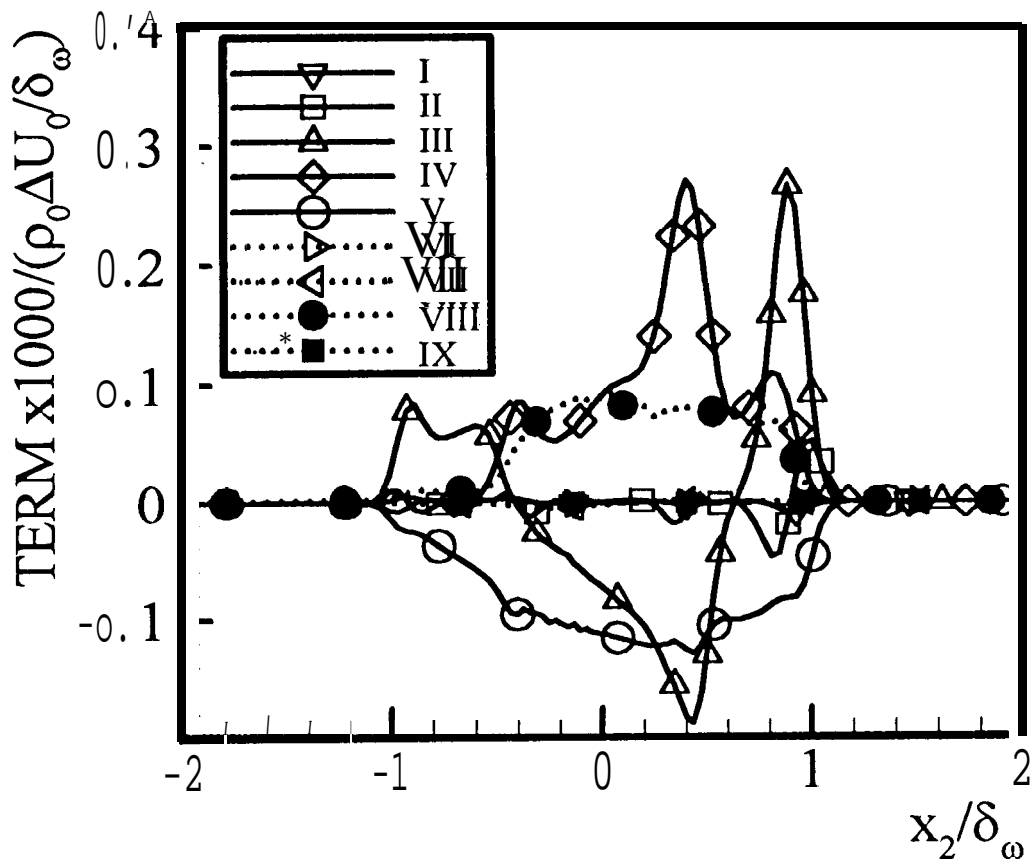


Figure 3c

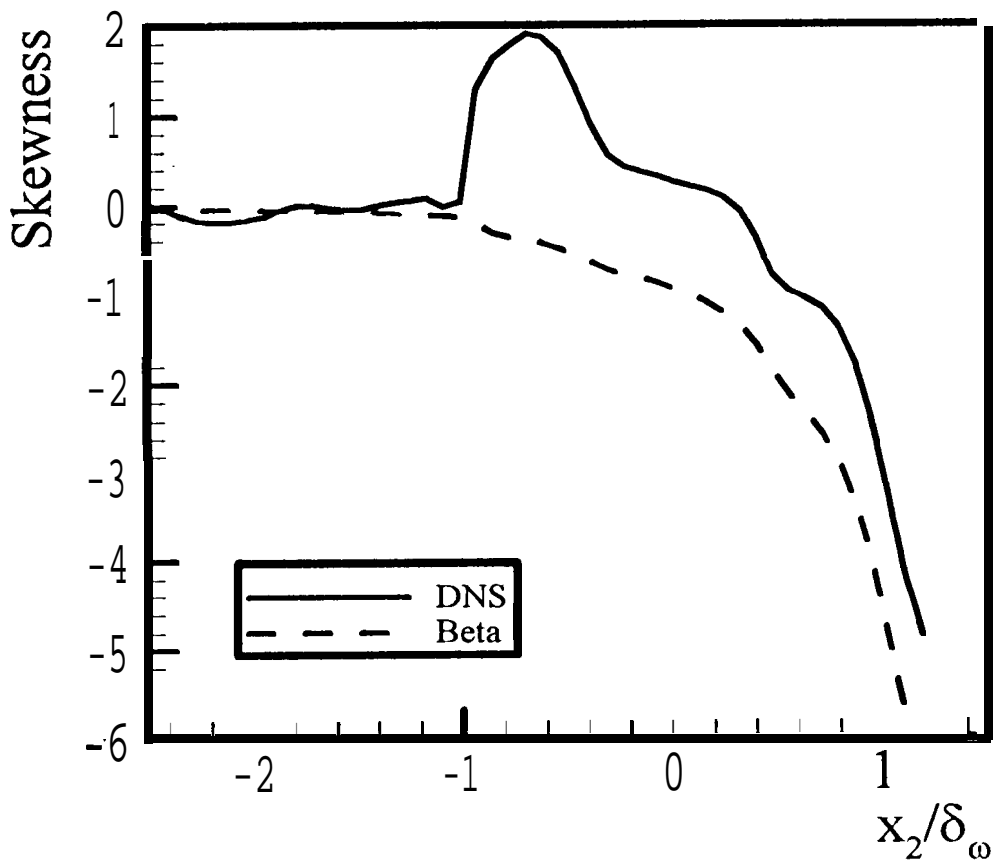


Figure 4a

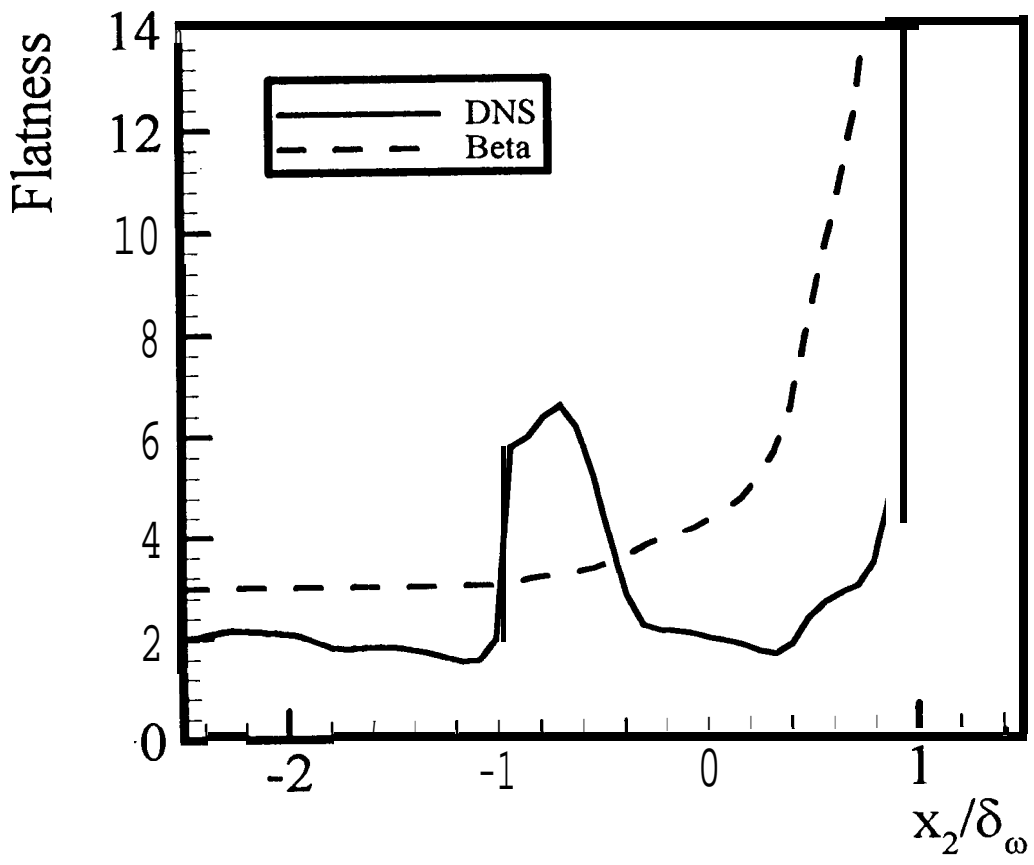


Figure 4b

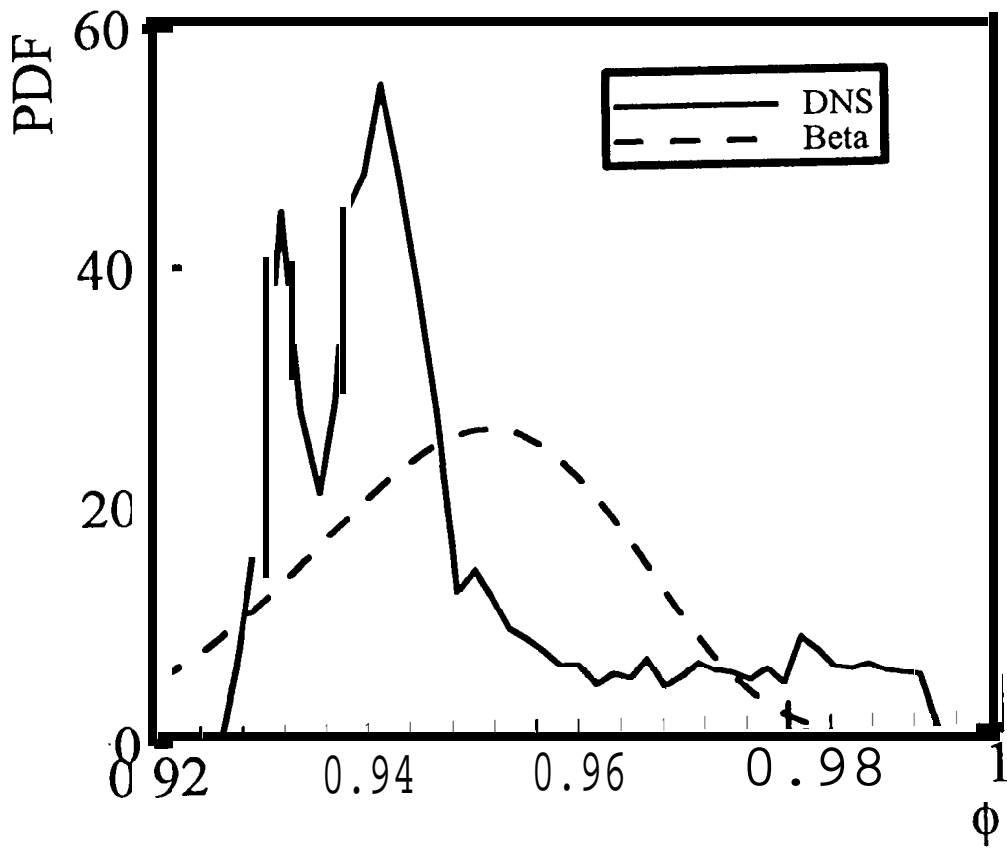


Figure 5