

**Computational Modeling of Low-Mach-Number  
High-Atwood-Number Turbulent Mixing (C4)**

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**Introduction**

One Dimensional Turbulence (ODT) is a stochastic model which tries to capture the essence of turbulent combustion: fully resolved molecular fluxes within a turbulent flow. To do this task a three dimensional velocity vector is described along a line (assumed to be the inhomogeneous direction in a temporal or spatially developing flow). Molecular processes are solved numerically and the turbulent flow effects of compressive strain rate and entrainment are accomplished with rearrangement events which are called the eddies. Upon random selection of an eddy length and location, guided by an assumed probability distribution, the proposed eddy energy is used to determine the eddy time scale, or frequency. This time scale is compared with an event rate distribution using a Bernoulli trial process; the eddy acceptance probability is kept low by the choice of the eddy time step so that the probability of more than one eddy occurring at one time vanishes. The action of the eddy is to rearrange all quantities within the eddy length – this is done by compressing the spatial scale to one-third of the eddy length, making two copies of the compressed result and placing them to fill out the eddy domain, the middle copy is then reversed. This triplet map will make a sawtooth curve out of a region with a linear gradient. Repeated application of the triplet map, at random locations, will generate a lognormal distribution of gradients.

In addition to the triplet mapping the eddy exchanges energy (energy flux) in the temporal (spatial) flow to mimic the pressure-strain-rate effects in turbulence. Using available direct numerical simulations (DNS) of Navier-Stokes turbulence in two shear flows, planar shear layer and planar wake, we have calibrated the ODT model by setting one rate term in order to match the temporal growth rate found in the DNS simulations. Comparison of first, second and third order turbulence quantities reveals nice agreement considering the simplicity of the ODT assumptions (Kerstein *et al.*, 2001).

New ODT work considers the temporal and spatial planar mixing layers in which the density of one stream may be a thousand times larger than the density of the other stream. This density contrast is achieved within incompressible flow by using two species with different molecular weights.

In this presentation we compare the variable density temporal shear with recent DNS compressible simulations by Pantano and Sarkar (2002). The spatially evolving ODT results are compared with the experiments performed by Brown and Roshko (1974). These experiments approximate incompressible flow while the DNS temporal simulations with density ratios up to eight were done with a convective Mach number of 0.7.

### ODT Flow Equations

We achieve variable-density, incompressible flow by using two species which have different molecular weights. The number density is constant and pressure gradients are also neglected (boundary layer approximation). We apply ODT to a shear layer which evolves in time (temporal) or in space (spatial) and conservation of streamwise momentum yields different governing equations between these two cases. The streamwise momentum in two dimensions is

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2}{\partial x} + \frac{\partial \rho uv}{\partial y} = vis$$

where  $vis$  is the viscous term. In the temporal case this reduces to  $\partial \rho u / \partial t = vis$  and there is no convective velocity, that feature is accomplished by the eddies. In steady spatial flow the momentum relation reduces to

$$\frac{\partial \rho u U}{\partial x} + \frac{\partial \rho u V}{\partial y} = vis$$

where  $U, V$  are the convection velocities with  $U = u$ , but  $V \neq v$  because convection is accomplished by the eddies. Thus, in the spatial case it is the flux of momentum which is conserved while in the temporal it is the momentum itself which is conserved. To mimic pressure scrambling of turbulence we exchange kinetic energy among the vector components in the temporal flow, but we exchange kinetic energy flux in the spatial flow, that is, exchange  $\rho u^2 U$  with  $\rho v^2 U$  and  $\rho w^2 U$ .

### Time Developing Flow Equations

The ODT velocity components on the 1D domain are denoted  $v_i(y, t)$ ,  $i = 1, 2, 3$ , where  $y$  (corresponding to  $i = 2$ ) is the domain coordinate. These velocities do no convection, convection is done by the eddies. The number density is constant (incompressible flow), but in a binary mixture with unequal molecular weights, the mass and momentum fluxes are not zero when the species gradient is not zero.

#### Density diffusion:

$$\frac{\partial \rho}{\partial t} = \kappa \frac{\partial^2 \rho}{\partial y^2}.$$

#### Momentum:

$$\frac{\partial \rho v_i}{\partial t} = \mu \frac{\partial^2 v_i}{\partial y^2} + \kappa \frac{\partial}{\partial y} v_i \frac{\partial \rho}{\partial y}$$

### Spatially Developing Flow Equations

Each ODT realization is a steady, planar flow. The streamwise advecting velocity  $U$  is the same as  $v_1$ , while the lateral advecting velocity  $V$  is different from  $v_2$ . This distinction is made because the  $v_i$  velocities are regarded as being storage of kinetic energy, and this energy is displaced by the eddy mappings. Therefore, the  $v_i$  velocities are not convective but evolve formally as passive scalars advected by  $U$  and  $V$  and diffused by viscosity.

#### Continuity:

$$\frac{\partial \rho U}{\partial x} + \frac{\partial \rho V}{\partial y} = 0$$

#### Density diffusion:

$$\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} = - \frac{\partial}{\partial y} \frac{\kappa}{\rho} \frac{\partial \rho}{\partial y}$$

note: incompressible flow has zero volume flux, and the mass average velocity is the sum of volume flux  $V'$  plus the diffusion flux,  $V = V' - (\kappa/\rho)(\partial \rho / \partial y)$ .

#### Momentum:

$$\frac{\partial \rho v_i U}{\partial x} + \frac{\partial \rho v_i V}{\partial y} = \mu \frac{\partial^2 v_i}{\partial y^2}$$

## Temporal Shear Layer

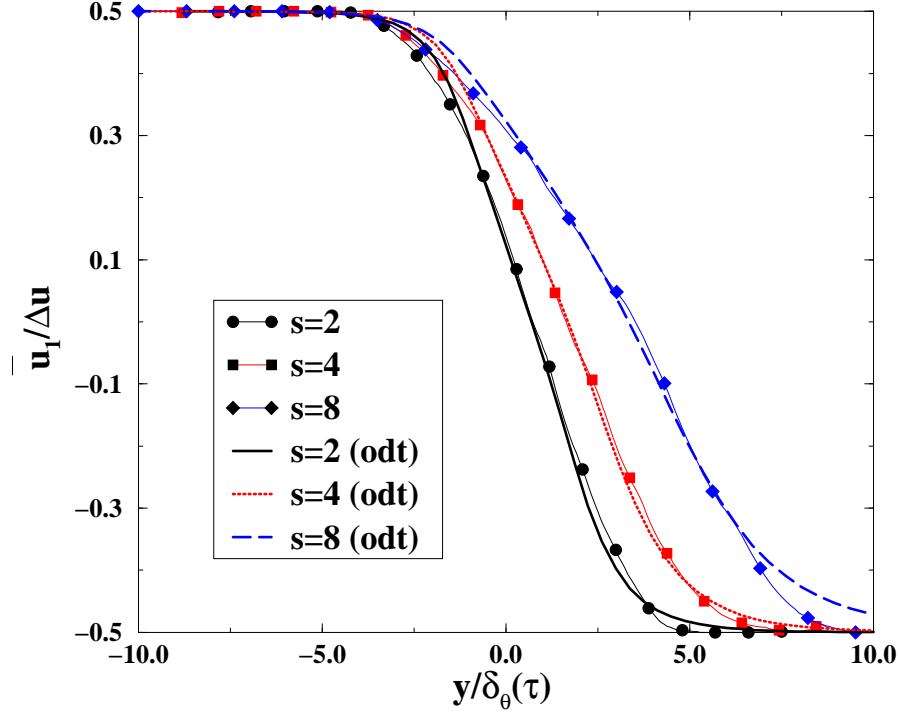
In our ODT temporal shear layer the one-dimensional line is in the lateral direction and we impose streamwise boundary velocities of  $U_1 = 0.5$  for  $y > 0$  and  $U_2 = -0.5$  for  $y < 0$ . We normalize velocities with  $\Delta U = U_1 - U_2$  and set  $\rho_2 = s\rho_1$  with  $\rho_1 = 1$ . With incompressible flow there is no equation of state.

Pantano and Sarkar (2002) have performed compressible DNS of the temporal shear layer using an ideal gas with constant specific heats, dynamic viscosity, thermal conductivity and diffusion. The energy equation is expressed as a dynamical equation for the pressure. Reference values are:  $L_o, \rho_o, p_o, U_o$  with the condition that  $\gamma Ma_o^2 = 1$  leading to  $p_o = \rho_o U_o^2$ . The convective Mach number is  $M_c = \Delta U / (c_1 + c_2)$ . The average density is fixed to unity  $\rho_o = (\rho_1 + \rho_2) / 2 = 1$  with  $s = \rho_2 / \rho_1$  and  $s \geq 1$  (by symmetry the flow with  $s = 1/s$  is the same flow). Their flow is periodic in the spanwise ( $z$ ) and streamwise ( $x$ ) directions while a free boundary is used in the lateral direction ( $y$ ). The initial conditions include broadband fluctuations, isotropic turbulence spectrum, in the shear region with an initial turbulence intensity of ten percent. They computed with convective Mach numbers of 0.3, 0.7 and 1.1 with a density ratio different from unity only in the 0.7 case.

The ODT parameters are those developed in the constant density work (Kerstein *et al.*, 2001), no new parameters were needed to include variable density, only the specification of a diffusivity was required. With constant dynamic viscosity  $\mu$ , the diffusivity is  $D_{12} = 0.6\mu((\rho_1 + \rho_2)/(\rho_1\rho_2))$ . The ODT mean streamwise velocity and density profiles agree with the DNS results ( $s = 1, 2, 4, 8$ ) and the ODT results indicate a reduced growth rate with increasing density ratio, similar to the behavior of the compressible layer. The ODT turbulent kinetic energy production, dissipation and transport have a peak amplitude which is about twice that of the compressible results. Future ODT work which includes a compressible velocity component may show that this amplitude difference is a compressibility effect.

## Temporal Shear Layer

Comparison with Compressible DNS,  $M_c = 0.7$



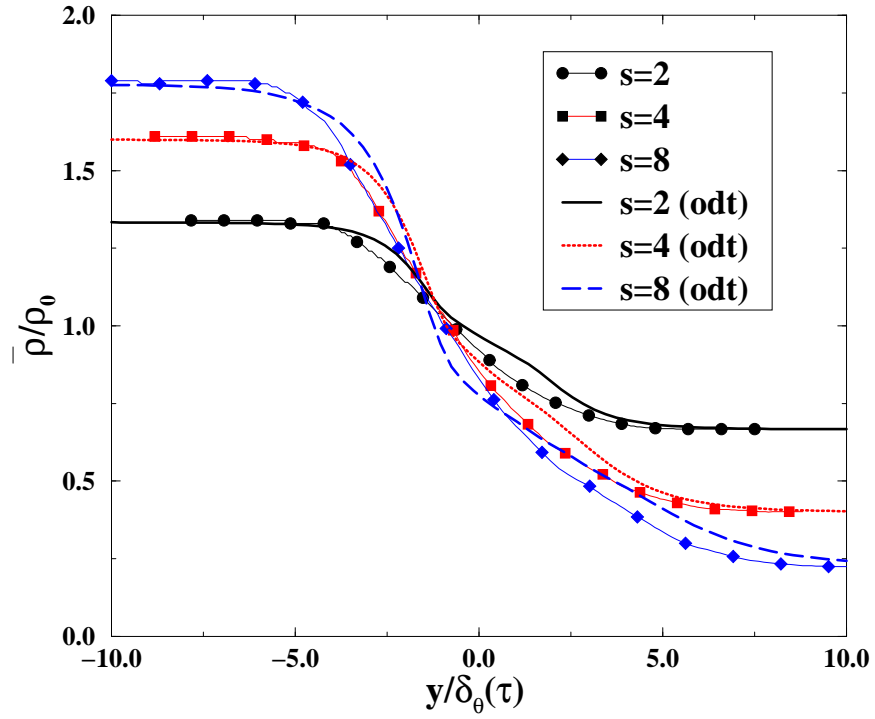
Mean streamwise velocity  $u$  from Pantano & Sarkar (JFM).

Momentum Thickness (Favre velocity:  $\tilde{u} = \overline{\rho u} / \bar{\rho}$ )

$$\delta_\theta = \frac{1}{\rho_o \Delta U^2} \int \bar{\rho} (u_1 - \tilde{u})(\tilde{u} - u_2) dy$$

## Temporal Shear Layer

Comparison with Compressible DNS,  $M_c = 0.7$



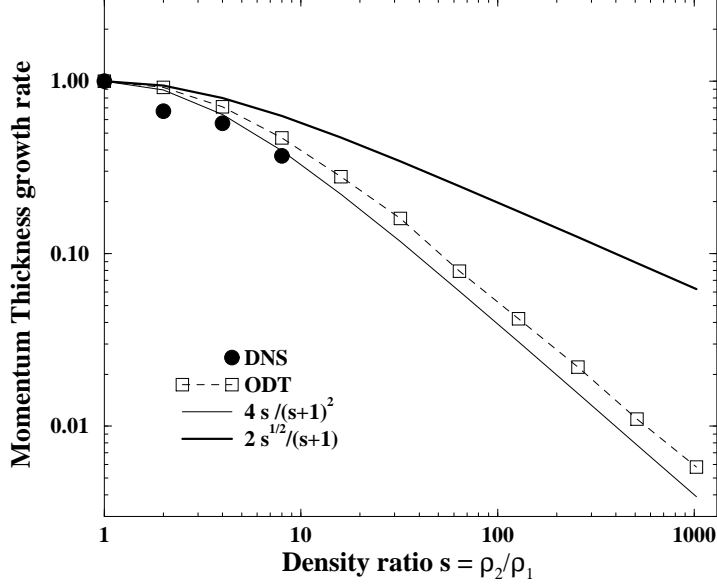
Mean density  $\rho$  from Pantano & Sarkar (JFM).

## Temporal Shear Layer

Comparison with Compressible DNS,  $M_c = 0.7$

### Pantano & Sarkar, $Mc = 0.7$

Table 9:  $\delta(s)/\delta(1)$  (Circles)



Momentum Thickness  $\delta_\theta$  growth rate from Pantano & Sarkar (JFM).

$$\delta_\theta = \frac{2}{(\rho_1 + \rho_2)(\Delta U)^2} \int \bar{\rho}(u_1 - \tilde{u})(\tilde{u} - u_2) dy$$

Favre velocity:  $\tilde{u} = \overline{\rho u} / \bar{\rho}$

Ramshaw (2000) has presented a model of shear layer growth, which when only the Kelvin-Helmholtz instability is active becomes

$$h \approx \Delta U t \frac{\sqrt{\rho_1 \rho_2}}{(\rho_1 + \rho_2)}$$

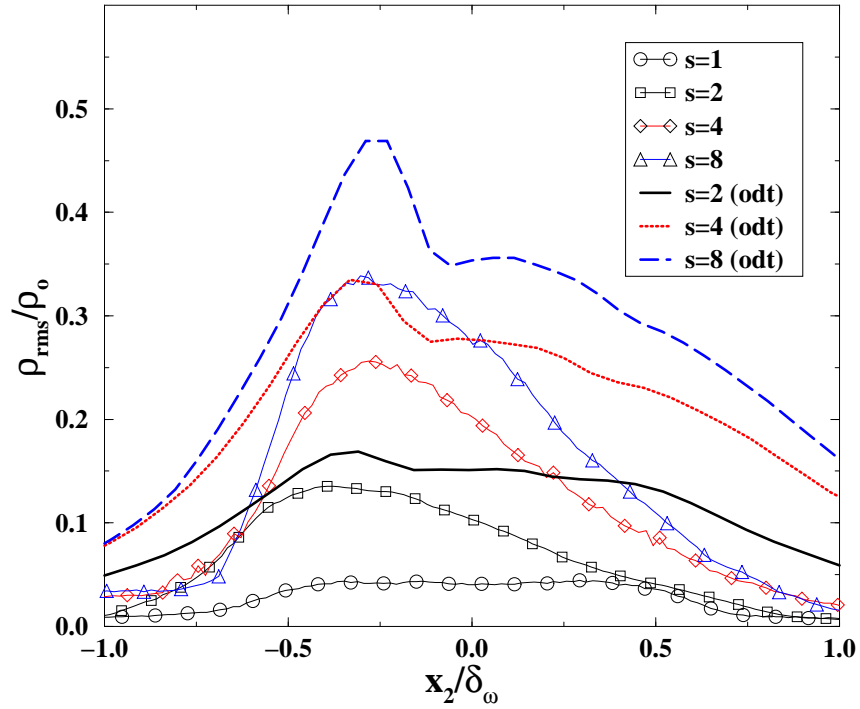
however, the ODT results indicate that the square of the density term is a better approximation

$$h \approx \Delta U t \frac{\rho_1 \rho_2}{(\rho_1 + \rho_2)^2}$$

which, with density ratio  $s = \rho_2/\rho_1$  gives the  $s/(s+1)^2$  effect shown in the figure above. Of course, being unit-less, there is no way to determine the exponent of this term by scaling laws.

## Temporal Shear Layer

Comparison with Compressible DNS,  $M_c = 0.7$



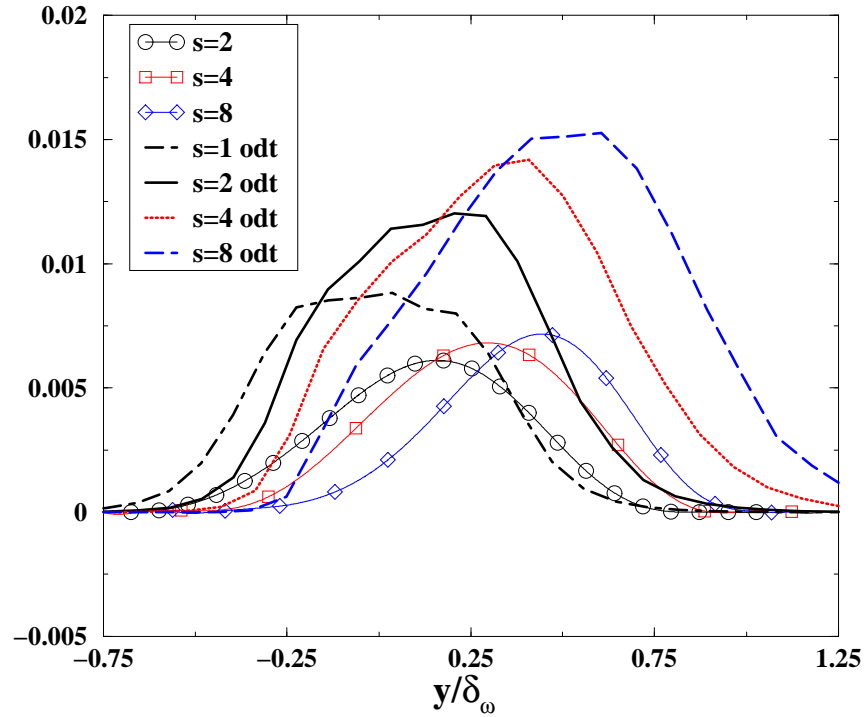
Density rms versus vorticity thickness  $\delta_\omega$   
(from Pantano & Sarkar, JFM)

Vorticity Thickness  $\delta_\omega = \Delta U / (\partial u / \partial y)_{max}$



## Temporal Shear Layer

Comparison with Compressible DNS,  $M_c = 0.7$

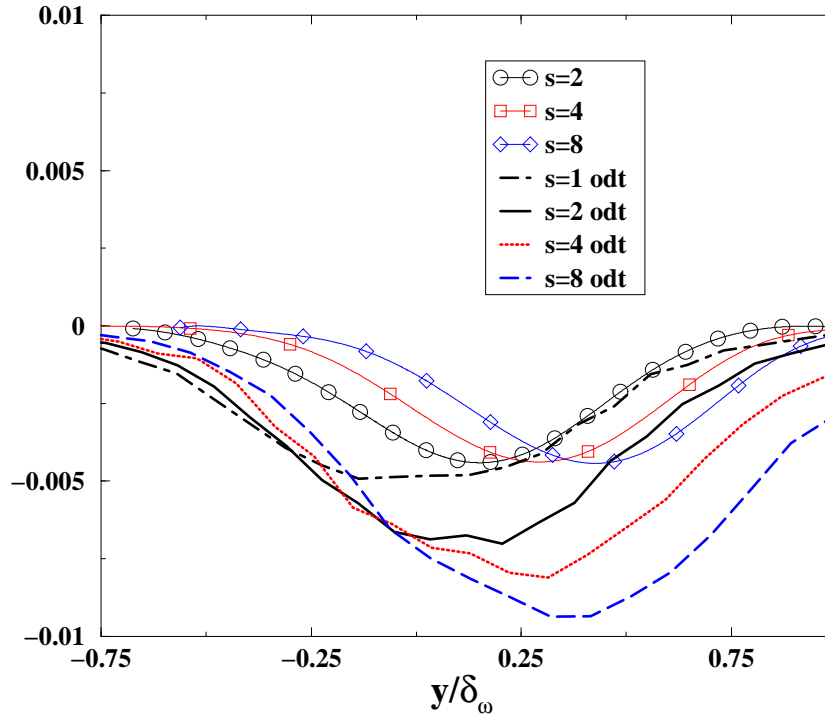


Turbulent kinetic energy production versus vorticity thickness  $\delta_\omega$   
(from Pantano & Sarkar, JFM)

Vorticity Thickness  $\delta_\omega = \Delta U / (\partial u / \partial y)_{max}$

## Temporal Shear Layer

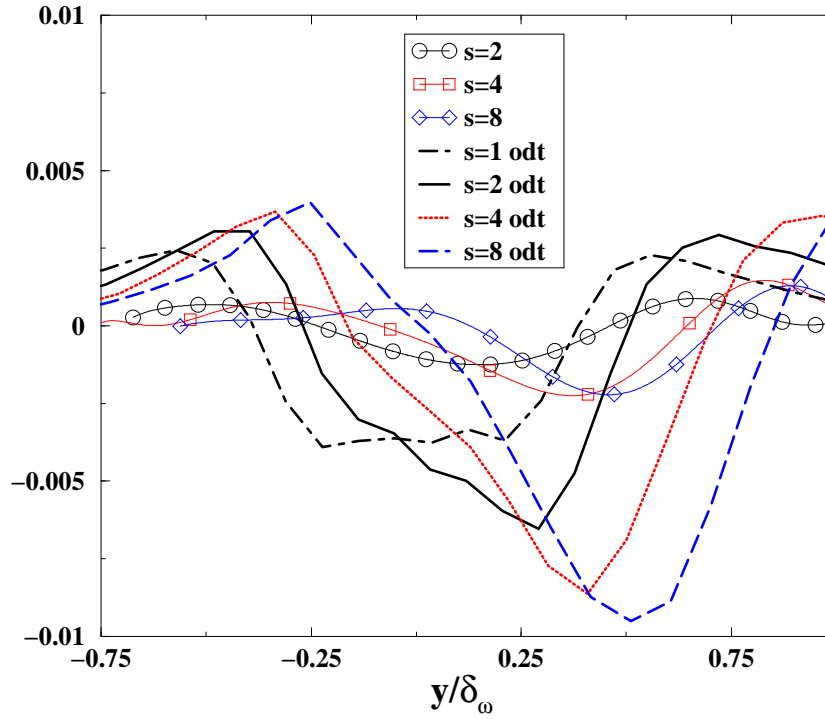
Comparison with Compressible DNS,  $M_c = 0.7$



Turbulent kinetic energy dissipation versus vorticity thickness  $\delta_\omega$   
(from Pantano & Sarkar, JFM)

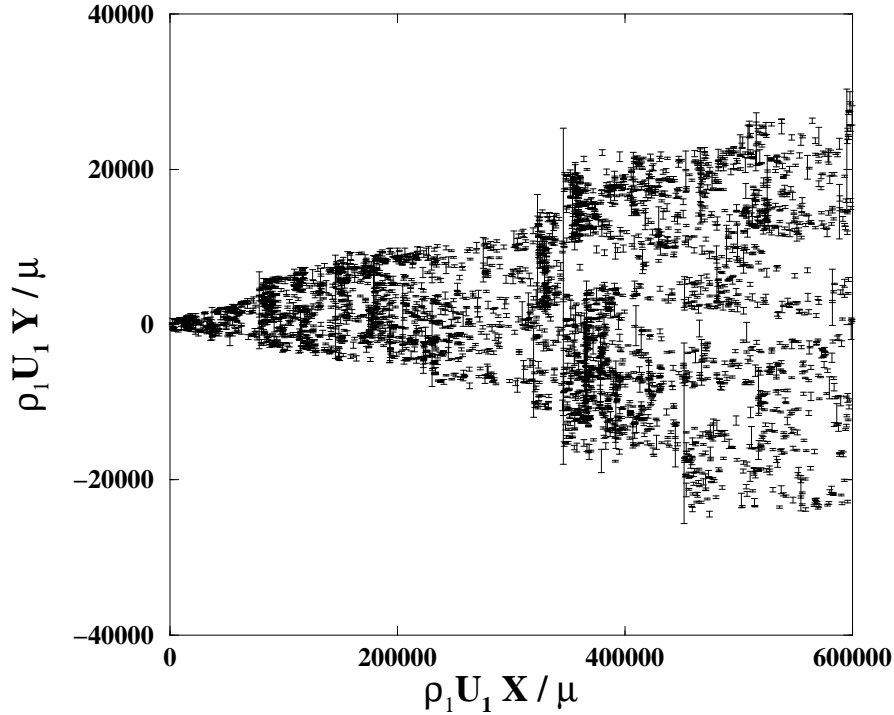
## Temporal Shear Layer

Comparison with Compressible DNS,  $M_c = 0.7$



Turbulent kinetic energy transport versus vorticity thickness  $\delta_\omega$   
(from Pantano & Sarkar, JFM)

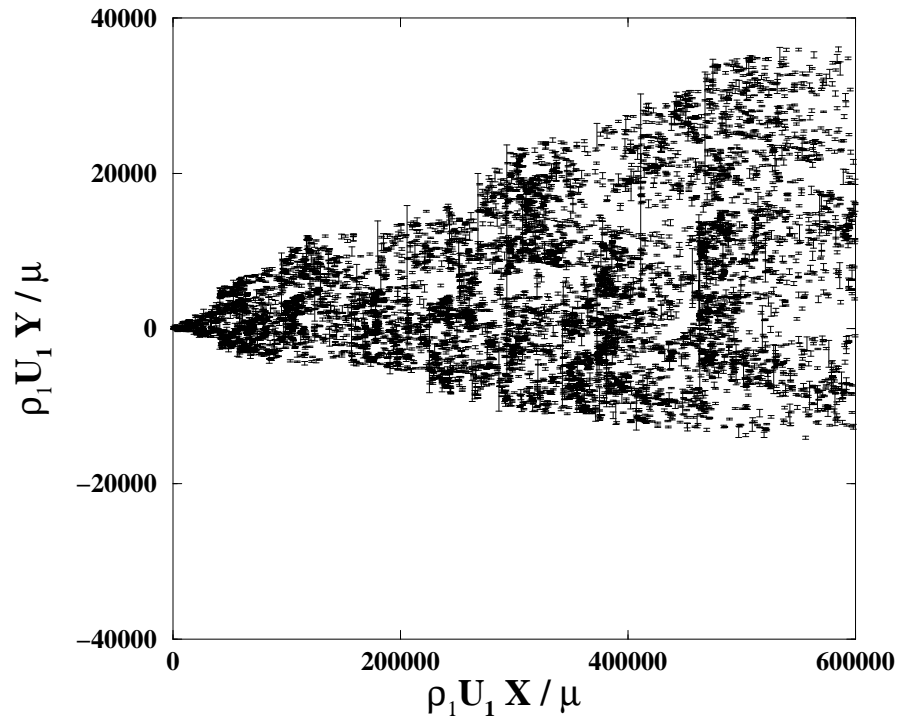
## SPATIALLY DEVELOPING SHEAR LAYER



The density ratio is unity  $s = 1$ , the upper flow has  $U_2 = 0.38$  and the lower flow has  $U_1 = 1$ , the Reynolds number is comparable to the experimental value.

One ODT realization is shown by drawing vertical lines corresponding to the eddy length and location. To be accepted the eddy energy, given by velocity component in the direction of the ODT line, combined with the eddy length must give a time scale which is smaller than the viscous time scale for that eddy length. An additional barrier to accepting an eddy is examination of eddy segments, each segment is one-third of the eddy, if any segment fails to be acceptable then the eddy is rejected. In this manner an eddy may protrude into the quiet freestream and thus cause an abrupt growth in the layer thickness. Notice the increased eddy activity downstream of the larger eddies, the larger eddy has enhanced the local shear which favors smaller eddies – thus forming a cascade of shear to small length scales.

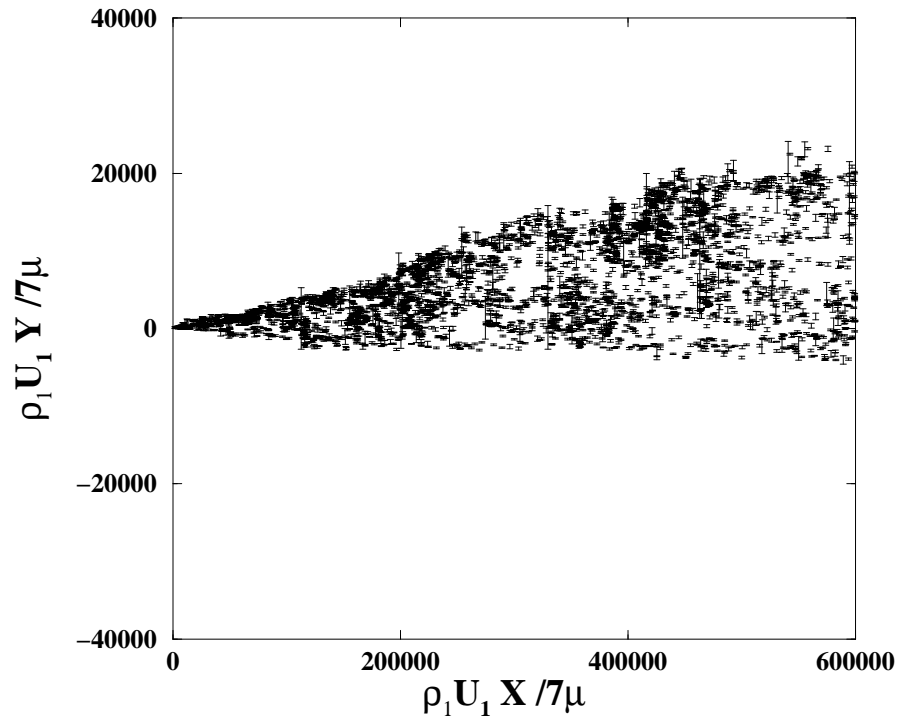
## SPATIALLY DEVELOPING SHEAR LAYER



The density ratio is  $s = 7 = \rho_2/\rho_1$ , the upper flow has  $U_1 = 1$  and the lower flow has  $U_2 = 0.38$ .

Notice that the spreading of the eddies into the lower flow, which has the larger inertia, is reduced by comparison with the upper flow.

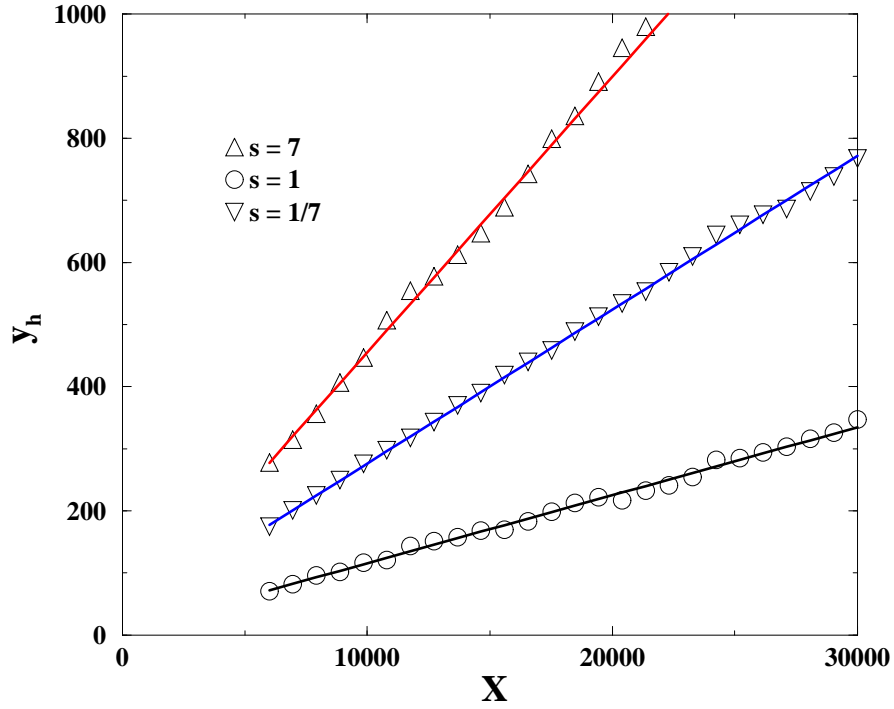
## SPATIALLY DEVELOPING SHEAR LAYER



The density ratio is  $s = 1/7 = \rho_2/\rho_1$ , the upper flow has  $U_2 = 0.38$  and the lower flow has  $U_1 = 1$ .

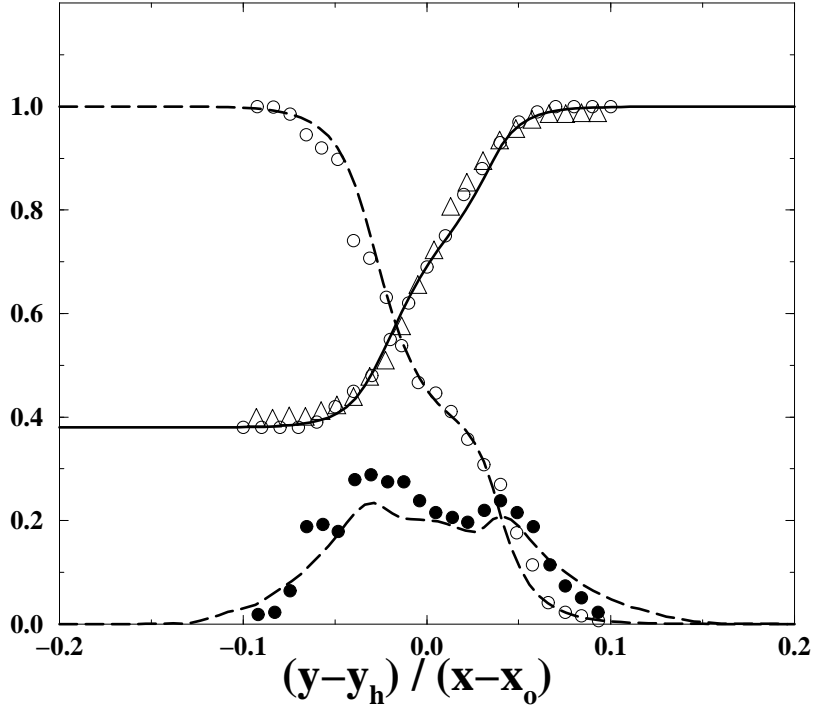
Notice that the faster flow which now has the larger inertia has very few eddies, and the overall growth rate is much less than when the denser flow is the slower stream (previous case with  $s = 7$ ).

## SPATIALLY DEVELOPING SHEAR LAYER



With each density ratio  $s = 7, 1, 1/7$ , one thousand realizations are used to determine mean profiles. An origin in the lateral direction is determined by the location where the Favre velocity equals the mean of the freestream velocities,  $\tilde{u} = (U_1 + U_2)/2$ , this defines  $y_h$ . The symbols denote  $y_h$  locations and the lines are least square fits which determine the virtual origin  $x_o$  and the growth rate. The lateral profiles will be shown as a function of the similarity coordinate  $(y - y_h)/(x - x_o)$ . In the spatial units shown here the dynamic viscosity has the value of  $1/20$ .

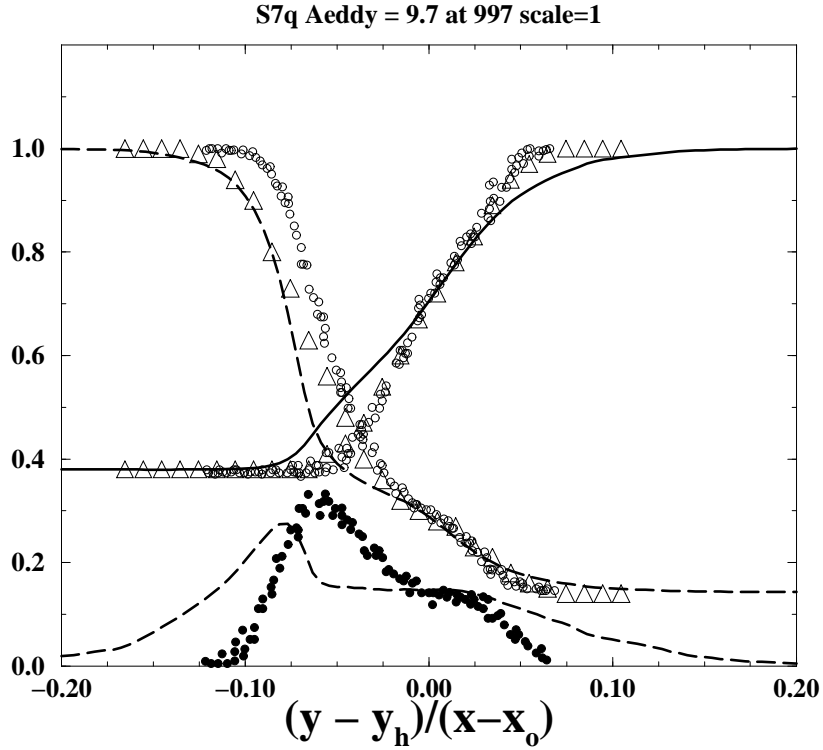
## SPATIALLY DEVELOPING SHEAR LAYER



Lateral profiles of velocity (ODT, solid line) and concentration and concentration rms values (ODT, dashed lines) with constant density  $s = 1$ ; the open triangles are from Brown & Roshko (velocity only) and the circles are from Konrad (velocity and concentration, open circle and concentration rms, filled circle). The ODT and Konrad's results have been scaled to match the velocity integral thickness of Brown & Roshko; this sets the eddy rate constant in the ODT simulations (which is used in the other density cases) and requires a factor of 0.7 times Konrad's lateral coordinate values. The velocity is reduced by the maximum velocity.

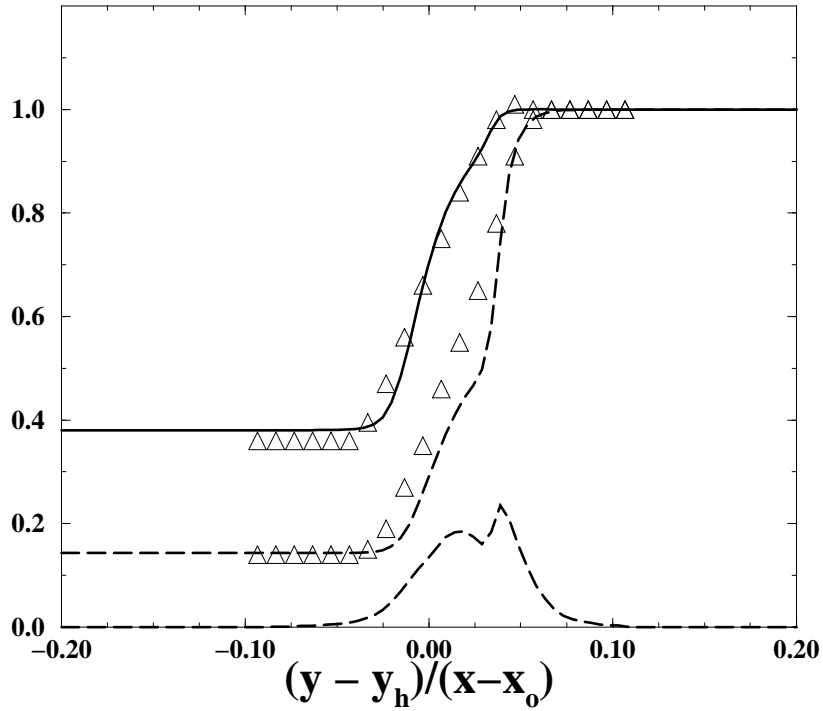


## SPATIALLY DEVELOPING SHEAR LAYER



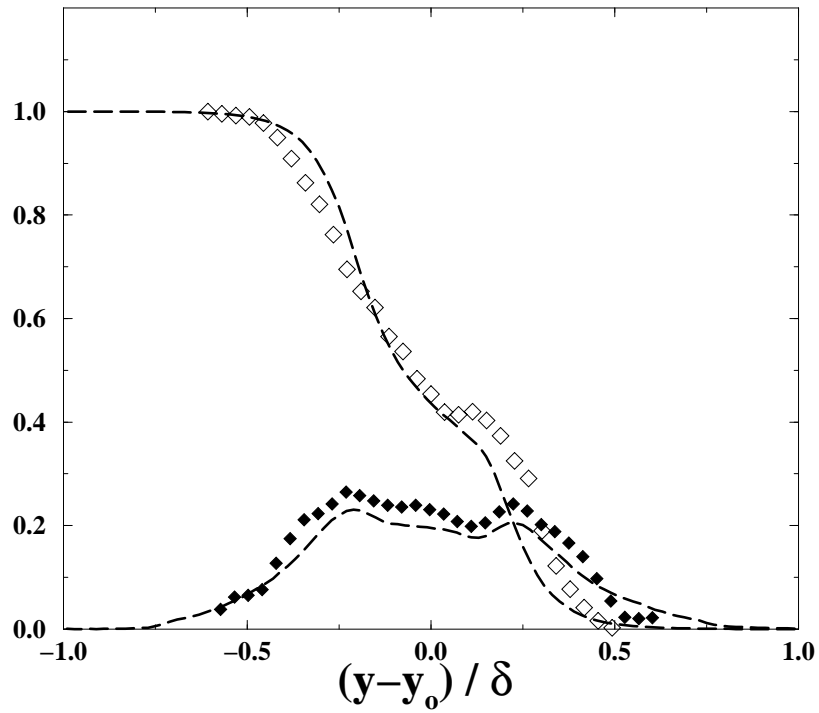
Lateral profiles of velocity (ODT, solid line) and density and rms density values (ODT, dashed lines) with density ratio  $s = 7$ ; the open triangles are from Brown & Roshko (velocity and density only) and the circles are from Konrad (velocity and density, open circle and rms density, filled circle). The lateral scale factors are the same as given in  $s = 1$  results; the density, and its rms, are normalized by the maximum density.

## SPATIALLY DEVELOPING SHEAR LAYER



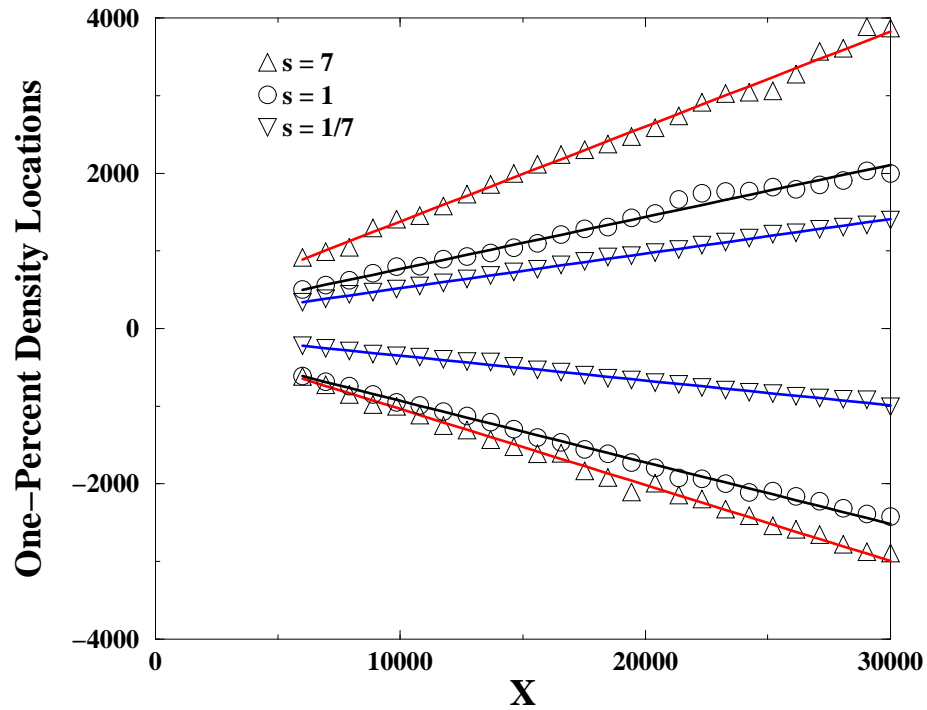
Lateral profiles of velocity (ODT, solid line) and density and rms density values (ODT, dashed lines) with density ratio  $s = 1/7$ ; the open triangles are from Brown & Roshko (velocity and density only). The lateral scale factors and normalizations are the same as given in  $s = 7$  results.

## SPATIALLY DEVELOPING SHEAR LAYER



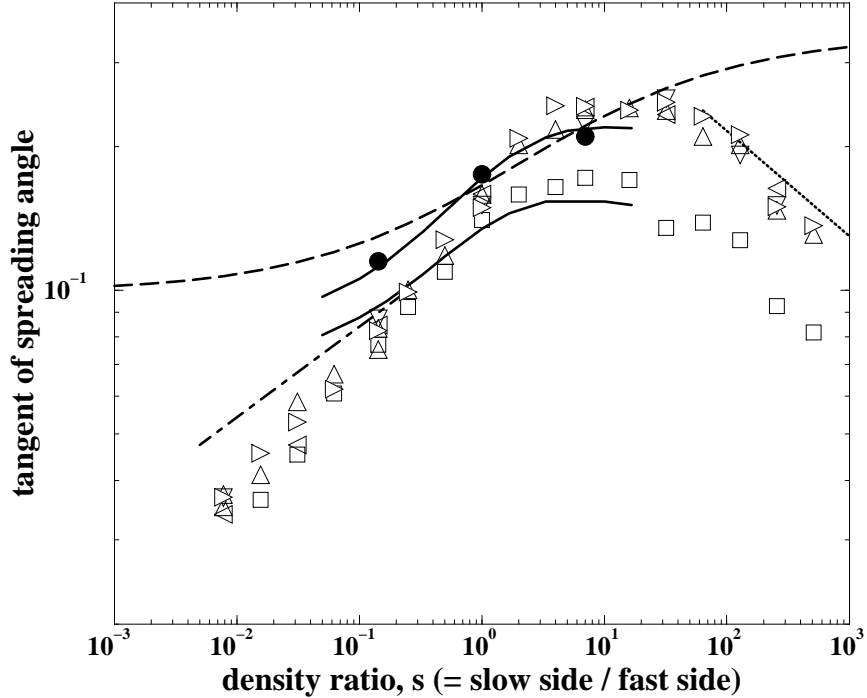
Concentration, and its rms, in constant density flow, velocity ratio of 0.4 (Pickett and Gandhi, Phys. Fluids, 2002, symbols) and ODT (dashed lines). Lateral scaling is from the concentration one-percent distance  $\delta$ , the lateral origin is the mean of those locations. The high speed stream is at positive  $y$  values.

## SPATIALLY DEVELOPING SHEAR LAYER



With each density ratio  $s = 7, 1, 1/7$ , one thousand realizations are used to determine mean profiles. The symbols denote the locations where the concentration is at a one-percent difference from its freestream value. The lines are least-square fits and the slope differences give the density growth rate.

## SPATIALLY DEVELOPING SHEAR LAYER



Density growth rate as a function of density ratio  $s$  and velocity ratio  $r = U_2/U_1$ . The ODT simulations have been matched to the experimental velocity integral thickness at  $s = 1$ ,  $r = 0.38$ , no other adjustments have been made for other density ratios or the other velocity ratio. The visual growth rate from Brown & Roshko (their figure 7) are given by the filled circles. The model of Dimotakis is the dashed line, while the two solid lines are given by the laminar stability of a compressible boundary layer, recently computed by Sandham at velocity ratios of 0.38 (upper) and 0.48 (lower). The ODT results ( $r = 0.38$ , triangles and  $r = 0.48$ , squares) indicate a power-law behavior when  $s$  is very small and when  $s$  is large. Similar behavior has been found in round jets: Siebers has found an exponent of 0.19 over the range of  $0.005 < s < 0.24$  in spray jets and Witze has found an exponent of -0.22 over the range of  $1 < s < 7$  in gaseous jets. These exponents of 0.19 (dot-dash) and -0.22 (dotted) are shown above with amplitudes to allow comparison with the ODT behavior.

## Acknowledgments

We thank Professor Sarkar and Dr. Pantano for sharing their DNS results and thank Professor Sandham for providing the stability results. Discussions with Professor Roshko have been helpful. This work supported by the Division of Chemical Sciences, Office of Basic Energy Sciences, U. S. Department of Energy.

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