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ABSTRACT

During the second year of our investigation we have followed closely the schedule outlined in our renewal proposal and each item we worked on is described in details in the body of this annual progress report. We have done the flow visualization of the mixing layer undergoing rapid chemical reaction, set up the laser doppler anemometer and selected an appropriate seeding for velocity fluctuations measurements. The calculations predicting the gross features of the shear layer have been carried out.

Separate publications resulting in part from this research are:

- 1 - Chevray, R. and Venkataramani K. S. "Total Dispersion of a scalar quantity in turbulent Flow", *Physics of Fluids*, 22, 12, December 1979. (submitted with this annual progress report).
- 2 - Omer, S. and Chevray R. "Concentration Fluctuations Measurements by Fiber-Optics Probe", (Abstract only), presented at the 33rd Meeting of the American Physical Society, Nov. 23-25, 1980, Cornell Univ., New York.
- 3 - Chevray, R., "Entrainment Interface in Free Turbulent Shear Flows", Invited Review paper, Progress in Energy and Combustion Science, in press

I. Flow Visualization and Laser Doppler Velocimetry

Flow visualization has been carried out in the specially constructed wind tunnel in which we will make the measurements. In order to render visible the reaction zone, we have chosen the well documented reaction of NH_3 with HCl which gives a monodisperse white aerosol. Still photographs were taken and a typical one is shown in Fig. 1. Movie films have recently been taken for different velocity ratio. They will be analyzed in details before the end of the current period. From the photographs, the reaction zone is clearly visible, and the growth of the mixing layer is put in evidence. Of particular interest are the initial instability, the region of rapid growth (vortex pairing) and the final region of rapid mixing due to the three-dimensional instability and the bursting into turbulence.

A Disa model 55X modular laser doppler velocimeter system has been acquired for velocity fluctuation measurements. The light source is a 15mW type 124B Spectra Physics helium - neon laser operating at a wave length of 632.8nm. The laser beam passes through an optical system comprised of a 55x21 cover and retarder, a 55x29 beam splitter, a 55x28 beam displacer, a 55x30 backscatter section, and a 55x51 planoconvex front lens, respectively.

Glass particles ranging in size from 1 - 5 μm diameter were obtained from Potter Industries, Inc., N.J., for use as seeding particles. Questions of following the flow with fidelity then arise. For a velocity error no greater than 1%, the criterion given by Maxumder and Kirsch is:

$$\frac{d^2}{36\nu} \left(2\frac{l_p}{l_f} + 1\right) \frac{u}{l} R_l^{1/2} \leq \frac{1}{74}$$

where l_p = particle density

l_f = fluid density

u = turbulence intensity

d = particle diameter

l = typical length scale for flow

Using this criterion, we should use glass particles of .34 μ m diameter (or 0.5 μ m PVC particles); above these dimensions, the lower scales of turbulence would be cut off as the particles would not follow the gas stream. Other criteria used in the selection of the particles as far as materials were concerned are: the inertness of particles in O_3 and NO, their resistance to "powder-compacting" or agglomeration and the necessity of not being too small in order to avoid molecular slip. With use of PVC particles, the first of these difficulties is avoided, the second is expected to be manageable, while the third is also expected to be small. Molecular slip will not present a real problem since this corresponds to very small particle diameter of about 0.1 μ m. Through experimentation with PVC particles of 0.5 μ m size, we have found the signal quality to be very good from those scatterers.

II. Calculations of the reacting turbulent mixing layer

The calculations of the mixing layer have been done by using the probability density function approach. The mean velocity and turbulence fields are determined by the mean momentum equations and the k- ϵ turbulence model. The equations are solved in their

boundary-layer form by a finite difference method. The concentrations of the reactants and products are determined from a model equation for the joint pdf of two scalars. Finally, the calculations were carried out by S. Pope as a consultant who has a working program to solve the pdf equation by a Monte Carlo method.

The mixing layer is shown in Fig. 2 with a velocity difference between the two streams

$$\Delta U = U_1 - U_2$$

The width of the mixing layer at any axial location is characterized by

$$\delta(x) = y_{0.9} - y_{0.1}$$

where $y_{0.9}$ and $y_{0.1}$ are defined by reference to the profiles of the mean axial velocity $\langle U(x,y) \rangle$:

$$\langle U(x, y_{0.9}) \rangle = U_2 + 0.9\Delta U ,$$

and

$$\langle U(x, y_{0.1}) \rangle = U_2 + 0.1\Delta U .$$

A normalized cross-stream coordinate η is introduced

$$\eta = (y - 1/2(y_{0.9} + y_{0.1}))/\delta$$

and the normalized axial velocity is

$$\hat{U}(x, \eta) = (U(x, y) - U_2)/\Delta U .$$

Note that, by definition,

$$\hat{U}(x, 1/2) = 0.9$$

and

$$\hat{U}(x, -1/2) = 0.1 .$$

A finite-difference method [1] is used to solve the boundary-layer equations for $\hat{U}$ and for the turbulent kinetic energy k and the dissipation ϵ . The turbulent viscosity is given by

$$\mu_T = C_\mu k^2 / \epsilon$$

where $c_\mu = 0.09$. The k - ϵ model is used in its standard form [2]

with the standard model constants: $C_{\epsilon 1} = 1.45$, $C_{\epsilon 2} = 1.90$, $\sigma_k = 1.0$, $\sigma_\epsilon = 1.3$.

Sufficiently far downstream of the splitter plate, the flow becomes self-similar so that $\hat{U}(x, \eta)$ and $d\delta/dx$ become independent of x . Then U and the spreading rate $d\delta/dx$ depend only upon the velocity ratio U_2/U_1 . Figure 2 shows the self-similar velocity profiles given by the k - ϵ model for velocity ratios $U_2/U_1 = 0.1, 0.3$ and 0.6 . The spreading rates are $d\delta/dx = 0.113, 0.0715$ and 0.0326 respectively. These values are in good agreement with experimental data (see Rodi).

In the subsequent calculations, it is assumed that the velocity and turbulence fields are self-preserving. This may not be the case for the experiment, but, without detailed knowledge of the initial conditions, it is the best assumption to make. Further, the k - ϵ model can be expected to be accurate only for fully-developed, high Reynolds number flows. Consequently, even if the initial conditions were known, the model may not produce an accurate description of the subsequent development of the flow.

Four trace species are involved in the reaction which is assumed to be irreversible:

The single major species is N_2 . Let m_α be the mass fraction of species α , W_α be the molecular weight and z_α is defined by

$$z_\alpha = m_\alpha / W_\alpha .$$

Assuming the molecular diffusivities Γ of the species are equal, the transport equations can be written

$$L(z_{NO}) = -S,$$

$$L(z_{O_3}) = -S,$$

$$L(z_{O_2}) = S,$$

and

$$L(z_{NO_2}) = S$$

where S is the reaction rate (kg moles/kg/s) and L is the linear differential operator

$$L = D/Dt - \Gamma \nabla^2 .$$

In the high and low-speed streams (denoted by 1 and 2), the boundary conditions are

	<u>high-speed</u>	<u>low-speed</u>
z_{NO}	$(z_{NO})_1$	0
z_{O_3}	0	$(z_{O_3})_2$
z_{O_2}	0	0
z_{NO_2}	0	0

where $(z_{NO})_1$ and $(z_{O_3})_2$ are the concentrations of the inlet streams,

Because the four species transport equations are linearly dependent, they can be replaced by just two equations -- one for a conserved scalar f and the other for a non-dimensional product

concentration $c \equiv z_{\text{NO}_2} / (z_{\text{O}_3})_2$:

$$L(f) = 0, \quad (f)_1 = 1, \quad (f)_2 = 0$$

$$L(c) = S / (z_{\text{O}_3})_2, \quad (c)_1 = 0, \quad (c)_2 = 0.$$

In terms of $\alpha \equiv (z_{\text{NO}})_1 / (z_{\text{O}_3})_2$ and $\beta \equiv (z_{\text{O}_3})_2 / (z_{\text{N}_2})_2$, the species concentrations are

$$z_{\text{NO}_2} = z_{\text{N}_2} \beta c,$$

$$z_{\text{O}_2} = z_{\text{N}_2} \beta c,$$

$$z_{\text{O}_2} = z_{\text{N}_2} \beta (1-f-c),$$

and

$$z_{\text{NO}} = z_{\text{N}_2} \beta (\alpha f - c).$$

The reaction rate is given by

$$S = \rho k_f z_{\text{NO}} z_{\text{O}_3},$$

where the rate constant $k_f = 9.6 \times 10^6 \text{ m}^3 / (\text{kg mole s})$. Making use of the perfect gas law

$$P/\rho = z_{\text{N}_2} RT,$$

and defining

$$\omega \equiv P k_f / (RT),$$

we obtain

$$S / (z_{\text{O}_3})_2 = \beta \omega S^*(f, c),$$

where

$$S^*(f, c) = (\alpha f - c)(1 - f - c) .$$

Thus c satisfies the transport equation

$$L(c) = \beta \omega S^*(f, c) .$$

At atmospheric temperature and pressure $\omega = 4 \times 10^5 \text{ s}^{-1}$.

Since all the species concentrations are related to c and f , a complete statistical description of the scalars in a turbulent flow is provided by the joint pdf of f and c , $p(\tilde{f}, \tilde{c}, \underline{x}, t)$. The pdf is defined so that $p(\tilde{f}, \tilde{c}) d\tilde{f} d\tilde{c}$ is the probability that f and c are in the ranges

$$\tilde{f} < f < \tilde{f} + d\tilde{f}$$

and

$$\tilde{c} < c < \tilde{c} + d\tilde{c} .$$

For two-dimensional boundary-layer flows, the modelled joint pdf equation used previously by Pope (1980) is

$$\langle U \rangle \frac{\partial p}{\partial x} + \langle V \rangle \frac{\partial p}{\partial y} = \frac{\partial}{\partial y} \Gamma_T \frac{\partial p}{\partial y} + \frac{\partial}{\partial \tilde{c}} \{ p \beta \omega S^*(\tilde{f}, \tilde{c}) \} + \omega_T E(\tilde{f}, \tilde{c}) ,$$

where

$$E(\tilde{f}, \tilde{c}) = 4 \int \int p(\tilde{f} + \tilde{f}^*, \tilde{c} + \tilde{c}^*) p(\tilde{f} - \tilde{f}^*, \tilde{c} - \tilde{c}^*) d\tilde{f}^* d\tilde{c}^* - p(\tilde{f}, \tilde{c}) .$$

The convection terms on the left-hand side of the equation are exact as is the reaction term. The first term on the right-hand side represents transport by the turbulent velocity fluctuations and is modelled by gradient diffusion: Γ_T is the turbulent diffusivity. The final term represents molecular mixing which is modelled by Curl's model. It is assumed that the Reynolds number is high so that the rate of molecular mixing is given by the turbulent frequency ω_T .

The joint pdf equation is now cast in dimensionless form.
 (Note that here U_1 not ΔU is used as the normalising velocity).
 The normalised axial and cross stream coordinates are

$$x^* \equiv x\beta\omega/U_1$$

and

$$\eta \equiv y/\delta.$$

It is assumed that the velocity and turbulence fields are self-similar so that

$$\delta = x(d\delta/dx) = x\sigma.$$

The following normalised quantities are now defined

$$\langle U(x,y) \rangle = U^*(\eta) U_1,$$

$$\langle V(x,y) \rangle = V^*(\eta) U_1,$$

$$\Gamma_T(x,y) = \Gamma_T^*(\eta) U_1 \delta,$$

$$\omega_T(x,y) = \omega_T^*(\eta) \delta/U_1,$$

and

$$p(\tilde{f}, \tilde{c}, x, y) = p^*(\tilde{f}, \tilde{c}, x^*, \eta).$$

The transformed pdf equation is

$$x^* \sigma U^* \frac{\partial p^*}{\partial x^*} + (V^* - \eta \sigma U^*) \frac{\partial p^*}{\partial \eta} =$$

$$\frac{\partial}{\partial \eta} \Gamma_T^* \frac{\partial p^*}{\partial \eta} + x^* \sigma \frac{\partial}{\partial \tilde{c}} (p^* S^*(\tilde{f}, \tilde{c})) + \omega_T E(\tilde{f}, \tilde{c})$$

The significance of this equation is that U_1 , U_2 , β and ω do not appear, even in a dimensionless group. The fluid mechanical quantities U^* , V^* , Γ_T^* , ω_T^* and σ are determined by the velocity ratio U_2/U_1 alone. The chemistry enters through the source term

$$S^*(\tilde{f}, \tilde{c}) = (\alpha \tilde{f} - \tilde{c})(1 - \tilde{f} - \tilde{c}),$$

which depends on the conditions only through the concentration ratio α . Thus the solution to the normalised pdf equation depends only upon the two dimensionless ratios U_2/U_1 and $\alpha = (z_{NO})_1/(z_{O_3})_2$. The absolute value of the velocity U_1 and the concentration $\beta = (z_{O_3})_2/(z_{N_2})_2$

determine the absolute value of the downstream distance x ,

$$x = x^* U_1 / (\beta \omega).$$

The normalised pdf equation was solved by the Monte Carlo method for $0 \leq x^* \leq 900$. There were 22 finite difference modes across the flow and the pdf was represented by 100 elements at each mode. A total of 220 forward steps in the x^* direction were taken.

Results

The pdf equation was solved for $U_2/U_1 = 0.3$ and $\alpha = 2$. This could correspond to $U_1 = 5$ m/s, $U_2 = 1.5$ m/s and NO and O_3 concentrations of 0.2% and 0.1% respectively. In that case, the scaling is

$$x = 1.25 x^* \text{ (cms)}$$

The initial mixing layer thickness was set to 10^{-4} so that self-preservation was achieved by $x^* = 0.01$, well before reaction is significant.

Figure 4 shows the calculated profiles of $\langle c(\eta, x^*) \rangle$ for $0.1 \leq x^* \leq x^* \leq 900$. For $x^* \geq 100$, the profiles are virtually coincident indicating that chemical equilibrium prevails. Finite reaction rates are important in the region $0.3 \leq x^* \leq 10.0$ (i.e., $0.4 \text{ cms} \leq x \leq 12.5 \text{ cms}$ for the case given above).

In order to assess the effects of turbulent concentration fluctuations, calculations were made in which the fluctuations were

assumed to be zero, and hence the mean reaction rate is

$$\langle S^* (f, c) \rangle = S^* (\langle f \rangle, \langle c \rangle) .$$

The resulting profiles of $\langle c(\eta, x^*) \rangle$ are shown on figure 5. It may be seen that the values of $\langle c \rangle$ are typically 20% higher than in the pdf calculations. The largest difference may be observed to be near the maximum in $\langle c \rangle$ where the curvature in the profile becomes very large.

Returning to the pdf calculations, figures 6 and 7 show profiles of $\langle f'^2 \rangle$, $\langle c'^2 \rangle$ and the correlation coefficient

$$R_{cf} \equiv \langle c'f' \rangle \{ \langle c'^2 \rangle \langle f'^2 \rangle \}^{-1/2} ,$$

at $x^* = 3.0$ and $x^* = 300$. The profile of $\langle f'^2 \rangle$, which is independent of x^* , rises monotonically to its maximum and then decreases monotonically with increasing η . Some measurements show that near $\eta = 0$ there may be a minimum in $\langle f'^2 \rangle$. The present calculations do not exhibit this. The profiles of $\langle c'^2 \rangle$ have two maxima. As expected the values of $\langle c'^2 \rangle$ increase between $x^* = 3$ and $x^* = 300$; also the shape is little changed.

The correlation coefficient R_{cf} is virtually the same at $x^* = 3.0$ and $x^* = 300$. The absolute values of R_{cf} are surprisingly high on both sides of the mixing layer.

III. Conclusions:

The experimental techniques to be used to carry out the measurements have been developed both for the velocity and concentration fluctuation measurements.

The calculations of the reacting mixing layer indicate that the region of interest, where finite rates play a role, is $0.3 < x^* < 10.0$. With $U_1 = 5$ m/s, and an ozone concentration of 0.1% this range is $0.4 \text{ cm} < x < 12.5 \text{ cm}$. For the conditions stated, at $x^* = 5$ the mixing layer thickness is just 4 mm and the ratio of laminar to turbulent viscosity is 0.1. It should be noted that the modelling assumes a high Reynolds number throughout and is likely to be inaccurate in the developing region. The profiles of $\langle c(\eta, x^*) \rangle$ shown on figures 5 and 6 also indicate that this quantity is not very sensitive to the modelling of the finite-rate reaction. The difference of 20% is most likely less than the combined uncertainty in the measurements and the turbulence mode. On the other hand, the profile of $\langle c'^2 \rangle$ and R_{cf} show some interesting trends which are likely to depend on the details of the modelling. These quantities, then, can be expected to be the more useful results of the experiment.

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Fig.1. Flow Visualization in the Mixing Layer ($r = \frac{U_1}{U_2} = 2.7$)

Fig. 2 Definition sketch

Fig. 3 Mean Velocity profiles
(normalized)

Fig. 4 Mean Concentration profiles
(normalized)

Fig. 5 Mean concentration profiles
without turbulent fluctuation

Fig. 6 Second order moment $x^* = 5$

Fig. 7 Second order moment $x^* = 300$.