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R. Chevray

State University of New York at Stony Brook
Long Island, New York 11794

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Abstract

This corresponds to the first year of our investigation into the interaction of chemical reactions and turbulence. During this time, we have a) completed construction of a special purpose wind tunnel, b) designed and constructed the fiber optics probe for concentration measurements, and c) set up the general method of attack on the theoretical front by first looking at the problem of total dispersion of a scalar in turbulent flows and independently setting up a scheme to model directly the equations describing the evolution of the probability density function of the species concentrations in the free shear layer. All the aforementioned tasks were performed on schedule according to the time chart originally proposed.

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1. Introduction

The need to study the interactions of chemical reactions and turbulence dictates the choice of a flow configuration which is simultaneously relevant to actual problems and simple enough so that results from it can be easily generalized. The two-dimensional free shear layer satisfies these requirements. For the reaction chosen, materials have been selected and a specialized wind tunnel built.

On the measurements front, we will use a novel, specially adapted absorption spectroscopic method to obtain simultaneous concentration fluctuations of two species. A special purpose probe which we fabricated is described in detail in part 4.

Finally, on the theoretical front, our efforts have been directed first at investigating the general problem of total dispersion of a passive scalar in turbulent flows and independently at setting up a scheme permitting a model to be made of the general equations of evolution of the probability density functions obtained from the conservation laws of a reactive flow system.

2. Wind Tunnel

The special purpose wind tunnel we built is shown in Figure 1 and consists of four basic sections: i) diffuser, ii) straight settling section, iii) contraction, and iv) test-section.

To avoid surface decomposition of ozone, the materials had to be chosen carefully. With this in mind, aluminum was selected as being the best readily available material with steel as the second best. Sections i - iii are made out of aluminum sheets $\frac{1}{4}$ " and 0.050" thick and secured together with threaded fasteners. Each of these sections have flanges at their ends for ease of assembly and of access to internal parts later on. When assembled, the wind tunnel has two separate compartments for the two streams, one nitric oxide diluted with nitrogen to up to 0.5% concentrations and the other ozone diluted with nitrogen to a maximum concentration of 0.1%. Both compartments are sealed from each other and from the atmosphere.

The diffuser section with an area ratio of 30 diverges at an angle of slightly less than 11° (total angle for each channel) so that there should be no boundary layer separation. A $100/\text{cm}^2$ wire-mesh screen is introduced in the mid-section of the diffuser that creates a negative pressure gradient to prevent any possible separation and also to damp the turbulence created at the inlet. In the straight section that follows, the two streams pass through a honeycomb (10 cells per cm^2) and three wire-mesh screens ($100/\text{cm}^2$) that serve to reduce the turbulence intensity of the flow to a minimum. The flow proceeds then to a contraction with a 4:1 area ratio where the steel splitter plate 1.6 mm thick tapers down to 0.05 mm at the beginning of the test section.

FIG. 1 WIND TUNNEL (SCALE 1.25)

The test section has aluminum top and bottom and side walls fabricated of plate glass to allow laser doppler velocity measurements as well as flow visualization in the visible range to be made. An identical section was made with plexiglas instead of plate glass for the side walls to permit flow visualization in the u.v. range to be made for ozone. The concentration fluctuations measurements using an absorption technique will be carried out by introducing the fiber optics probe, described in part 4, from the top. Both top and bottom have the flexibility to be flared to compensate for boundary layer growth (we estimate the boundary layer displacement thickness to be about 8 mm at the end of the test section for a Reynolds number of 40,000), so that we will effectively obtain a mixing layer with zero pressure gradient. The gases, after the test section, are exhausted into a specially fabricated section where they are collected before being passed through water to be absorbed.

The maximum velocities that we are planning to use are 5 m/s for nitro ϕ oxide stream and 2 m/s for the ozone side. Measurements will be taken for ratio of velocities between 0.1 and 0.6; a velocity of 5 m/s corresponds to a Reynolds number of 40,000 based on hydraulic diameter at the inlet of the test section.

3. Gas Delivery System

For the ($\text{NO} + \text{N}_2$) stream, with a maximum flow velocity of 5 m/s and a cross sectional area at the inlet of the test section equal to 187 cm^2 we have a flow rate (at 1 atm) equal to 94 l/s corresponding to a total volume of 141 m^3 for 150 s running time. On the ozone side, we plan on using a maximum flow velocity of 2 m/s corresponding to a flow rate at 1 atmosphere of 37 l/s; the resulting volume of the gases for 150 s running time at 1 atm is 5.6 m^3 of which .1% (5.6 l) is ozone.

The requirements for the NO side can be met without much complications since bottled nitric oxide is available commercially and can be mixed on line with nitrogen gas. The large flow rate of nitrogen gas is achieved by manifolding six "T" cylinders (301 ft^3 at 2,640 psi) of nitrogen gas using a two-row manifold TRB-2-6-580 and a high flow capacity pressure regulator 20-A-16, all manufactured by Linde Specialty gases and related products. The "prepurified" grade of nitrogen used has a minimum purity of 99.99% with a moisture content of less than 3 ppm.

For the slower ozone and nitrogen stream, we use a single row manifold SRB-2-3-580 and three "T" size bottles of "prepurified" nitrogen together with the high flow capacity pressure regulator 20-A-16 mentioned earlier. The ozone to be used in the experiment is produced by a Welsbach Model T-816 laboratory ozonator equipped with adjustable gas flow rate and pressure. The ozonator is supplied with pure oxygen from a Linde T cylinder containing 331 ft^3 of O_2 at 2640 psig with a minimum purity of 99.6% and a maximum moisture of 10 ppm. The maximum rate of ozone that can be produced in this manner is 7.4 standard liters per hour.

An optimum ozone concentration for the experiment is in the range 0.05 - 0.1% by volume in order to get a good signal intensity from the fiber-optics probe. This maximum of 0.1% is also much within the limit of 0.01 atm partial pressure for ozone, below which Shea* reports that no heat-release effects were noticeable in a similar experiment. In other words, a concentration of 0.1% ozone in mixture insures the dilution number $\Delta T/T = -\Delta\rho/\rho$ to be sufficiently small. Corresponding to this concentration, we need a mixture flow rate of 37.5 l/s, that is an ozone flow rate of 225 l/hr which is much greater than the production rate from the ozonator.

A scheme for storage of O_3 is therefore needed, capable of storing a total ozone volume of 5.6 l (for a 150 s running time). Since ozone is produced from oxygen at about 4% O_3 in O_2 by volume, we need to store a volume equal to 140 l. Two different schemes for the storage problem are presently under comparative evaluation. In the first approach, while running, the ozonator feeds the O_3 and O_2 mixture into a thick-walled, strong balloon at a pressure slightly higher than atmospheric. With the ozonator capacity of 7 liters of O_3 per hour, a one-hour run will produce the required 5.6 l of ozone. This ozone is later compressed into a standard gas bottle at about 2 atm pressure and delivered to the nitrogen main line through a sonic throat.

In the second scheme, the ozonator delivery line is connected to a compressor which brings the mixture to 5 atm (say) and fills a regular Linde T tank for storing high pressure gases. At 5 atm, the total gas

*J. Fluid Mechanics 81 (1977) pp. 317-333.

mixture stored is 250 liters of standard gas. With the ozonator rate, the tank therefore fills up in about 2 hours. This compressed mixture is then delivered in a manner similar to that described in the first scheme via a sonic throat.

As a comparason of the two methods, large amounts of ozone and oxygen will have to be stored at a high pressure in the second scheme which, although not impossible* is better avoided. The first scheme does not have these disadvantages, but its feasibility depends on obtaining a durable and safe balloon for storing ozone at atmospheric pressure. The required size is 150 l which is quite reasonable and currently work is under progress to obtain such a balloon.

*Waller & McTurk, J. Appl. Chem. 15 (1965) pp. 363-365.

4. Fiber Optics System

The technique used for monitoring concentration fluctuations is shown schematically in Figure 2. The components required for this have been specified to and built by Math Associates, Inc. The source of light being used is a 50W mercury short arc lamp operating on 50 VDC. The input assembly filters transmit the two required wavelengths 2537 Å and 4350 Å, for ozone--and nitric oxide--absorption measurements, respectively, which are conducted by optical cable, made of fused silica, that bears good transmission characteristics in the u.v. range, to the test section. The end of this cable, together with one end of the receiving cable forms the probe for concentration measurements.

The receiving cable leads to two silicon photodiodes through dual interference filter that detect the intensity of each of the two wavelengths transmitted through the measuring volume.

The reference channel, fabricated of the same material as the probe is illuminated by the same source above and serves to monitor any intensity fluctuations from mercury lamp due to arc instability and flicker.

The minimum concentration of ozone or nitric oxide detectable is determined from the relation

$$\ln \frac{I_0}{I} = \int_0^x \alpha [c] dx$$

where I_0 = intensity of beam at zero concentration of gas

I - intensity of beam at any concentration of gas

α = absorption coefficient

$[c]$ = concentration

x = path length.

1. TEST CHANNEL

2. REFERENCE CHANNEL

FIG. 2 OPTICAL SYSTEM (SCHEMATIC)

Thus for the ozone stream as an example, with $\alpha = 1.14 \times 10^{-17} \text{ cm}^2/\text{molecule}$ at 2537 Å, 0.1% concentration by volume corresponds to $2.7 \times 10^{16} \text{ molecules/cm}^3$ and I/I_0 to 0.72.

The absorption characteristics of the gases used is given in table 1 (for which 1830 Å is given as an alternative for possible detection of NO)

Table 1. Absorption coefficient ($\text{cm}^{-1}\text{atm}^{-1}$)

gas wavelength	O ₃	NO	NO ₂	O ₂
1830 Å	0.5	40	0.1	0.1
2537 Å	139	1	0.6	$\sim 10^{-5}$ very small
4350 Å	very small	very small	0.6	very small

From it, by ignoring electronic noise and absorption of trace impurities we estimate for ozone detection a signal to noise ratio

$$\frac{E_{\text{REF}} - E[\text{O}_3]}{E_{\text{noise}}} = 85.$$

Traces of certain oxides of nitrogen, principally N_2O_5 and N_2O are to be found in ozone sources such as the one we are using. Under typical conditions, the mole ratio of ozone to either one is of the order of 100 to 1 and this might have to be taken into account in a refined evaluation of the signal to noise ratio.

5. Theoretical Work

The first effort in this direction has been to look at the general problem of the dispersion of a scalar quantity in turbulent flow (corresponding to the case of fast reaction). The essential feature of this formulation is the consideration of the motion of the isoconcentration surfaces and explicit expressions (which check with earlier results by Saffman*) are obtained. A preprint of this work which was initiated under another sponsorship is appended to this report and has been published in the Physics of Fluids** (reprints will be forwarded as soon as they become available). On another aspect of our theoretical approach, we are modelling directly the equations derived for the p.d.f. evolution for the species concentration for the case of the shear layer.

*Saffman, P. G. Mecanique de la Turbulence, CNRS, Paris, 1962, p. 53.

**Chevray, R. and Venkataramani, K. S. Physics of Fluids 22, 12 (December 1979) 2284.

6. Efforts

The principal investigator spent 2 months full time during the summer of 1979 on this project as well as 20% time during the academic year starting September 1979. During the remaining of the current term, the principal investigator will spend 20% of his time as expected.

7. Conclusions

During this first year of our investigation into the interactions of chemical reactions and turbulence we have:

- a. designed and constructed a special purpose wind tunnel;
- b. designed and fabricated a fiber optics probe for simultaneous measurement of 2 species concentration fluctuations;
- c. obtained explicit results giving the total dispersion of a passive scalar quantity in turbulent flows (preprint attached) and set up a scheme to predict the evolution of the p.d.f. equations for species concentrations in our two-dimensional mixing layer.