The Role of Ventilation
15th AIVC Conference, Buxton, Great Britain
27-30 September 1994

Investigation of Effect of Tracer Species on Tracer Mixing Using CFD

S B Riffat, L Shao

Building Technology Group, School of Architecture,
University of Nottingham, NG7 2RD United Kingdom

SYNOPSIS

Tracer-gas techniques are widely used for measurement of airflow in buildings and their accuracy depends critically on the uniformity of tracer/air mixing. However, tracer mixing is still an unsolved problem and the effect of many factors remains unclear. This paper presents a study of the effect on mixing of tracer species. The investigation concentrated on tracer mixing involved in the decay technique, which is the most widely used version of the tracer gas method. The distribution and history of tracer concentration during air flow measurements were examined using Computational Fluid Dynamics (CFD). It was found that for single-zone tracer decay tests, three tracer gases, sulphur hexafluoride, nitrous oxide and carbon dioxide have virtually identical mixing patterns and thus there is no difference between them in terms of flow rate measurement results. However, for multi-tracer gas tests where there is interzonal tracer movement, the three tracer gases with different binary diffusivities exhibit significantly different mixing behaviour. In these situations, the choice of tracer will impact the accuracy of air flow measurement.

LIST OF SYMBOLS

A, B	Components A and B
C	Tracer concentration (%)
D	Molecular diffusivity (m^2/s)
k	Boltzmann's constant, 1.3805×10^{-25} (J/K)
M	Molecular weight (g/mol)
P	Pressure (Pa)
t	time (second)
T	Temperature (°C)
T_b	Normal boiling point (°C)
V	Velocity
V_b	Liquid molar volume at boiling point (m^3/mol)
ε	Characteristic energy parameter
Ω_D	Diffusion collision integral (dimensionless)
μ_p	Dipole moment (debyes)
σ	Collision diameter (m)

1. INTRODUCTION

Tracer-gas techniques[1-5] are widely used for building airflow measurements. However, they have a potential problem, i.e. the discrepancy between the less than perfect tracer mixing achieved in practical tests and the theoretical requirement of uniform tracer concentration within the test zone during the test. This requirement implies that the supply air entering the zone must instantly achieve uniform mixing with the air-tracer mixture in the zone. This is physically unsound and tracer mixing is still, in general, an unsolved difficulty.

The accuracy of tracer-gas methods has been the subject of much research. However, until recently it has been predominantly along the line of analysing the effect of measurement errors on the flow rate results. Such work provided information on acceptable measurement errors and elucidated the most error tolerating algorithm for flow rate derivation. These studies, by accepting the algorithms, implicitly assume that the tracer concentration is uniform

and errors arise solely from equipment or operators. They therefore did not address the crucial problem of mixing. More recently, the focus of research is starting to switch to the more fundamental study of factors affecting tracer mixing[6-9]. These are necessary in order to provide insight into the mixing mechanisms, based upon which, better mixing enhancement methods may be devised in the future. It has been shown that smaller building zones, lower air change rates and higher inlet airflow velocities have positive effects on tracer/air mixing and that there does not exist a universal critical value of air change rate below which satisfactory mixing is guaranteed. Nevertheless, many more questions regarding tracer mixing remain unanswered.

This paper presents a study of the effect of tracer species on mixing. It is usually assumed[1, 6] that tracer mixing is independent of the tracer species, which appears reasonable, given the always small proportions of tracer-gas in tracer-air mixtures. However, there is recent experimental evidence[8, 9] to contradict this assumption. In both studies, three different tracer-gases were used and these gave rise to different flow rate results for the same flow. This study examines this problem using an analytical/computational approach and the results were used to compare with previously obtained experimental findings.

2. COMPUTATION PROCEDURES

The CFD code FLUENT was used to solve the three dimensional Navier-Stokes equations and time dependent simulations were carried out to predict the transient tracer concentration variation.

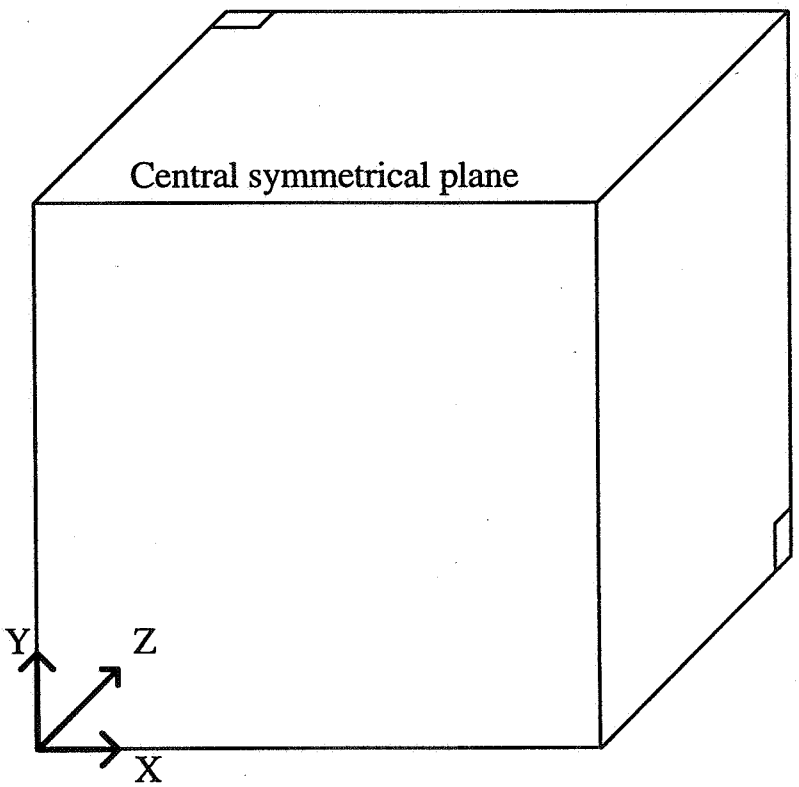

Fig. 1 Schematic of the computation domain.

The building zone used in this study is of cubic shape and measures 3m×3m×3m. The three-dimensional computational domain was selected in preference to the two-dimensional one, despite the penalty in CPU processing time. It is felt that in a two-dimensional domain, the air-stream from the inlet to the outlet will divide the domain into separate areas, isolating them from each other, resulting in mixing being artificially obstructed. The zone used in the computation is symmetrical about its central symmetrical plane. This fact was utilised to reduce the amount of computer storage and calculation required by including only one half of the zone in the computation domain (Fig. 1). As a consequence, the central symmetrical plane becomes one of the boundaries and the symmetrical boundary conditions were imposed, which assumes that the velocity component perpendicular to the plain is zero and all scalar gradients are zero. The supply air inlet for the room, as shown in Fig. 1, has a cross section 0.15m × 0.3m. The supply air stream enters the room perpendicular to the inlet at a uniform speed of 0.01 m/s. This resembles the magnitude of stack-driven natural convection between building zones and provides a bulk airflow rate of 1/3 ach. This velocity was selected to enable the computational assessment of tracer mixing in zones that are not saturated with fully developed turbulence. In situations where fully developed turbulence prevails, the mixing between air and different species of tracer will be identical. This is because molecular mixing which is species-dependent is several orders of magnitude weaker than turbulent mixing, the latter being dependent only on the flow properties. However it is rare to find fully developed turbulence in building air infiltration and ventilation. In the vast majority of cases, there is co-existence of turbulent areas and laminar areas or the flow is completely laminar. Thus there could be differences in terms of mixing between different species. The outlet for the exhaust air has the same shape and dimensions as the inlet and only half of both were included in the computation domain as is the case for the building zone.

Three tracer-gases, sulphur hexafluoride, nitrous oxide and carbon dioxide, were used to examine the effect of tracer species on mixing. Diffusion of one gaseous species into another is governed by

$$J = -D\frac{dC}{dx},$$

for one-dimensional diffusion and the equivalent equation for three-dimensional diffusion is very similar. Here J is the diffusion flux across unit area normal to the x-direction, $\frac{dC}{dx}$ is the concentration gradient and D is binary diffusivity. Binary diffusivity data for the three tracer-gases used in this computation were calculated based on molecular kinetics[10] as outlined in the following. The binary diffusivity of a two gaseous species (A and B) system is given by:

$$D_{AB} = 1.858\times10^{-3} T^{3/2} \frac{(\frac{1}{M_A} + \frac{1}{M_B})^{1/2}}{P\sigma_{AB}{}^2\Omega_D},$$

where

M = molecular weight, g/mol

D_{AB} = binary diffusivity, cm^2/s

T = temperature, K

P = pressure, atm

Ω_D is diffusion collision integral (dimensionless) which can be calculated using

$$\Omega_D = \frac{A}{T^{*B}} + \frac{C}{e^{DT^*}} + \frac{E}{e^{FT^*}} + \frac{G}{e^{HT^*}} + \frac{0.19\delta_{AB}^{\ 2}}{T^*} \qquad (1)$$

where A = 1.06036, B = 0.15610, C = 0.19300, D = 0.47635, E = 1.03587, F = 1.52996, G = 1.76474, H = 3.89411;

$$\delta_{AB} = (\delta_A \delta_B)^{1/2}$$

$$T^* = \frac{kT}{\varepsilon_{AB}}$$

$$\frac{\varepsilon_{AB}}{k} = (\frac{\varepsilon_A}{k}\frac{\varepsilon_B}{k})^{1/2}$$

$$\frac{\varepsilon}{k} = 1.18(1+1.3\delta^2)T_b$$

$$\delta = \frac{1.94\times10^3 \mu_p^{\ 2}}{V_b T_b}$$

σ_{AB} in equation (1) is defined by

$$\sigma_{AB} = (\sigma_A \sigma_B)^{1/2}$$

where σ is collision diameter with unit Å and is evaluated by

$$\sigma = (\frac{1.585V_b}{1+1.3\delta^2})^{1/3}$$

The binary diffusivities for sulphur hexafluoride-air, nitrous oxide-air and carbon dioxide-air at the temperature of 288K were calculated as 8.8532×10^{-6}, 1.35566×10^{-5} and 1.50348×10^{-5} m^2/s.

Single-tracer or multiple-tracer decay tests can be classified into two groups. Consider the simplest multiple-tracer decay tests: Two zones, A and B, are injected with tracers "a" and "b" respectively. During the test, fresh air from the outside environment and flow from zone B will mix with the tracer "a" and air mixture in zone A, diluting tracer "a". On the other hand flow from zone B also carries tracer "b" into zone A, increasing the "b" concentration there. These two distinct mixing situations occur in a similar way to zone B. Indeed, the two groups of mixing situation can be identified in all multiple tracer tests. The first type is referred to as type "aA" mixing and the second "bA" mixing. Mixing in all single-tracer decay tests and mixing of tracer "a" in zone A belong to the first type and mixing of tracer "b" in zone A belongs to the second.

In light of the above discussion, two groups of a total of six cases of tracer mixing were examined. In the first group, which corresponds to the "aA" type described above, the room was injected with one of the three tracers described above which then is mixed with the air in the zone to achieve a uniform concentration of 0.1%. As the test starts, fresh air enters the zone and the variation of tracer concentration distribution with time is recorded; The computation is halted when the accumulative air change reaches 1/3 ac. The same procedure is repeated for the other two tracer-gases and the three set of results are then compared to determine the effect of tracer species. The second group, corresponding to the "bA" type

mixing, of three cases was computed in a similar manner. The only difference is that the air in the zone at the start of the tests is fresh (free from tracers) while the supply air entering the zone had a uniform tracer concentration of 0.1%.

3. RESULTS AND DISCUSSION

Figs. 2, 3 and 4 are results from the first group of three cases. Fig. 2 shows the sulphur hexafluoride concentration distribution, by means of concentration contours, across the central symmetrical plane. This is a "snap-shot" at the end of the test when 1/3 air change has been accumulated. The concentration is measured as the ratio of the mass of the tracer to the mass of air. The values for the contours, in the order from upper-right to lower-left are, in equal steps, 9.93×10^{-4}, 9.41×10^{-4}, 8.89×10^{-4}, 8.36×10^{-4}, 7.84×10^{-4}, 7.32×10^{-4}, 6.80×10^{-4}, 6.27×10^{-4}, 5.75×10^{-4}, 5.23×10^{-4}, 4.70×10^{-4}, 4.18×10^{-4}, 3.66×10^{-4}, 3.14×10^{-4}, 2.61×10^{-4}, 2.09×10^{-4}, 1.57×10^{-4}, 1.05×10^{-4}, 5.23×10^{-5}, respectively. Figs. 3 and 4 are interpreted in the same way except that they show the concentration distribution of nitrous oxide and carbon dioxide, respectively. The distribution patterns show remarkable similarity. At any particular point on the plane the differences in concentration between the three tracer-gases are smaller than 5%. In fact, the similarity is repeated across the complete zone. These results show that the mixing between air and each of the three tracer-gases is virtually identical and that all three tracer-gases would yield the similar results when used in flow rate measurement.

Very different results emerge from the second group of three cases which correspond to the "bA" type mixing. The supply air has a uniform tracer concentration of 0.1% and the zone contains no tracer-gas at the start of the test. Fig. 5 shows the tracer concentration histories for sulphur hexafluoride, nitrous oxide and carbon dioxide at a spatial point with co-ordinates in x, y and z axes of 1.5, 1.5 and 1.0, respectively. The definition of the co-ordinate system is shown in Fig. 1. Large differences in concentration, especially between sulphur hexafluoride and the other two tracers, is evident and maintained for most part of the test duration. These differences are consistent with the fact that the binary diffusivities of nitrous oxide and carbon dioxide are much larger than that of sulphur hexafluoride. Obviously, the mixing performances of the three tracer-gases are significantly different, which is closely related to their widely differing molecular diffusion capacity.

The histories of concentration variation of the three tracer-gases at 19 other points, positioned throughout the domain, were also examined. The twenty points are classified into three groups according to the gaps between the concentration curves for the three tracers. In the first group, the curves for the three tracers virtually coincide; Sampling points where the gap, in terms of relative difference in concentration, averages up to 10% are assigned to the second group and those with gaps over 10% form the third group. For example, the sampling point for Fig. 5 belongs to group three. Among the 20 sampling points, there are 4 in group one, 7 in group two and 9 in group three. These results indicate that tracer-air mixing for sulphur hexafluoride, nitrous oxide and carbon dioxide are significantly different for "bA" type situations.

It has been explained previously that all single-zone tracer decay tests are associated with "aA" type tracer mixing and all multi-zone or multi-tracer decay tests involve "bA" as well as "aA" type mixing. It follows from the above results concerning the two mixing types that for single-zone tracer decay tests, there is no difference between the three tracer-gases, sulphur hexafluoride, nitrous oxide and carbon dioxide, in terms of results of flow rate

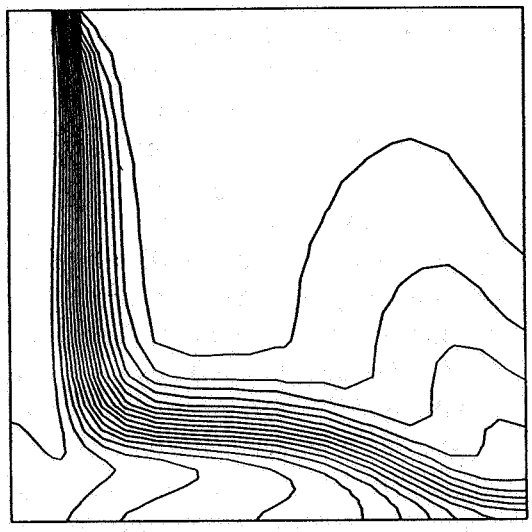

Figure 2. Concentration contours for SF_6 in the central symmetrical plane.

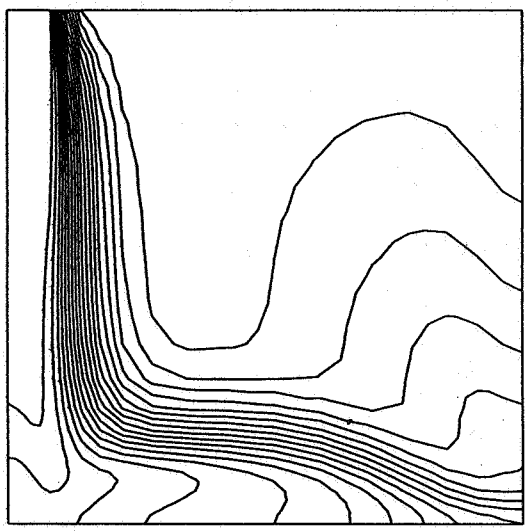

Figure 3. Concentration contours for N_2O in the central symmetrical plane.

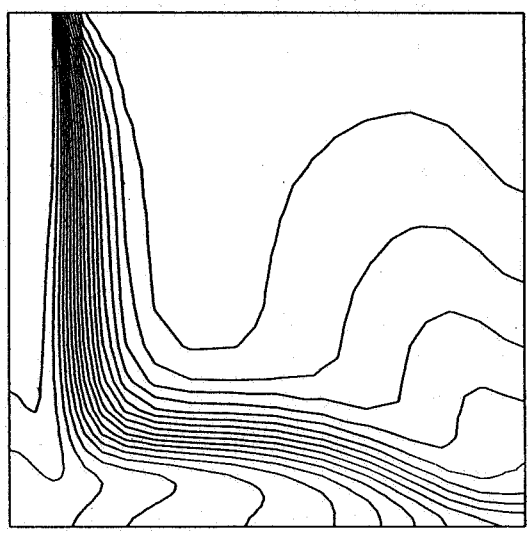

Figure 4. Concentration contours for CO_2 in the central symmetrical plane.

measurements. However, for multi-tracer-gas tests, the choice of tracer will impact the result of airflow measurement. This conclusion supports recent experimental findings by Kohal and Riffat[9] who revealed the significant effect of tracer species on flow rate measurement results. They revealed that nitrous oxide tends to perform better than sulphur hexafluoride, which is in line with the fact that the binary diffusivity of the former is significantly higher and that tracer concentration distribution results from this study show greater uniformity for the former. The results from this study also show that carbon dioxide tends to have better mixing than nitrous oxide and sulphur hexafluoride, as it has the highest binary diffusivity of the three tracer-gases. However, significant and variable background concentration and relatively poor detectability of carbon dioxide discourage its use as a tracer-gas. The level of detectability of carbon dioxide is around 3 and 7 orders of magnitudes lower than those of nitrous oxide and sulphur hexafluoride[1], respectively. As a result, 100 litres of carbon dioxide may need to be injected into a modest sized (3m×3m×3m) zone. Heating, cooking and breathing contribute to oscillation in background carbon dioxide concentration, causing uncertainty and inaccuracy in flow rate measurements. As a result, carbon dioxide may not perform as well as the other two tracers despite of its high diffusivity. This is borne out by recent experimental results[9].

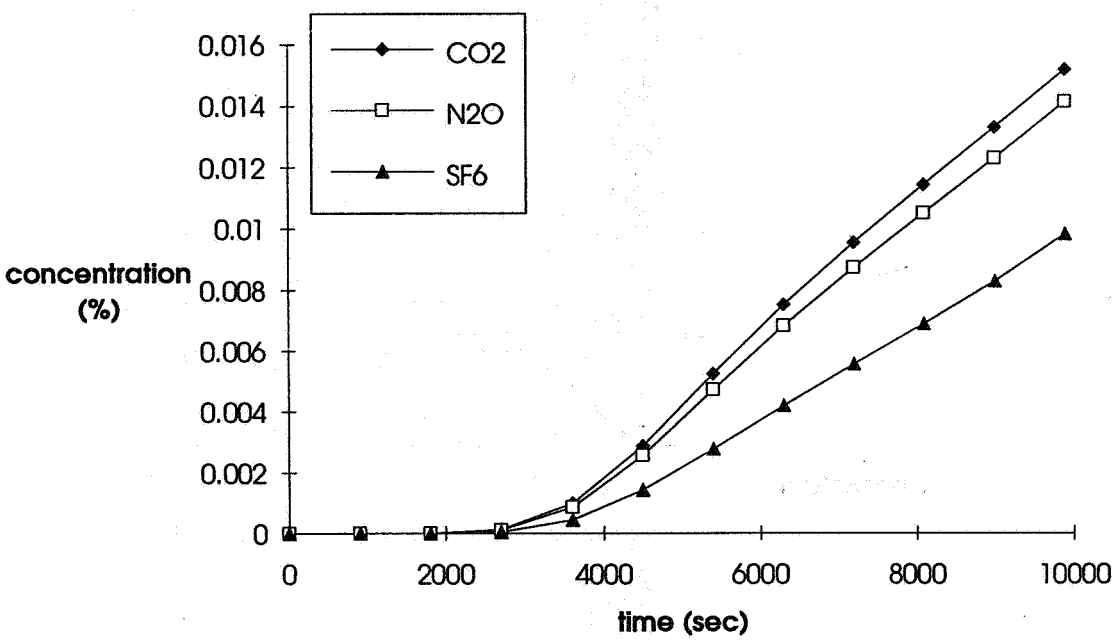

Figure 5. Concentration history for three tracer-gases.

4. CONCLUSIONS

The effect on mixing of tracer species has been examined using computational fluid dynamics. It was found that for single-zone tracer decay tests, three tracer-gases, sulphur hexafluoride, nitrous oxide and carbon dioxide have virtually identical mixing patterns and thus there is no difference between them in terms of flow rate measurement results. However, for multi-tracer-gas tests where there is interzonal tracer movement, the three tracer-gases with different binary diffusivities exhibit significantly different mixing behaviour. In these situations, the choice of tracer will impact the accuracy of airflow measurement. These conclusions support

recent experimental findings concerning the significant effect of tracer species on flow rate measurement results.

The sequence of the tracers, in the order of descending mixing power, is carbon dioxide, nitrous oxide and sulphur hexafluoride, which is a result of their different diffusivities, also in the same order. However, mixing power should be considered together with other practical factors when making a choice of tracer-gas. Use of carbon dioxide should be avoided despite of its high diffusivity because of its significant and variable background concentration and relatively poor detectability.

REFERENCES

1. Roulet, C. -A. & Vandaele, L., Airflow patterns within buildings: Measurement techniques. AIVC TN-34 (1991).
2. Wouters, P., l'Heureux, D. & Voordecker, P. The determination of leakages by simultaneous use of tracer gas and pressurisation equipment. *Air infiltration Review* **8**(1) 4-4 (1986).
3. Shao, L. & Howarth, A. T. Air infiltration through background cracks due to temperature difference. *BSER&T* **13**(1) 25-30 (1992).
4. Cheong, K. W. & Riffat, S. B., Perfluorocarbon tracer (PFT) for measurement of airflow in ducts. *BSER&T*, **17**(1) (1994).
5. Sherman, M. H. & Dickerhoff, D. J., A multi-gas tracer system for multizone air flow measurements. *ASHRAE/DOE/BTECC Symp. on Thermal Performance of External Envelopes of Buildings, Atlanta, USA* (1989).
6. Shao, L., Sharples, S. & Ward, I. C., Tracer gas mixing with air. *BSER&T*, **14**(2) (1993).
7. Alevantis, M. S. & Hayward, S. B., The feasibility of achieving necessary initial mixing when using tracer gas decay for ventilation measurement. *Proc. 5th Int. Conf. on Indoor Air Quality and Climate, Toronto, Canada,* 349-354 (1990).
8. Niemela, R., Lefevre, A., Muller, J.-P. & Aubertin, G., Comparison of three tracer gases for determining ventilation effectiveness and capture efficiency. *Roomvent'90, Oslo*, C-44 (1990).
9. Kohal, J. S. & Riffat, S. B., Computer modelling and measurement of airflow in an environmental chamber. *Proc. 14th AIVC Conference, Copenhagen, Denmark,* 421-431 (1993).
10. Fahien, R. W., *Fundamentals of transport phenomena.* McGraw-Hill, (1983).