Building and Environment, Vol. 23, No. 3, pp. 187–194, 1988.
Printed in Great Britain.

0360–1323/88 $3.00+0.00
Pergamon Press plc.

#3350

Error Analysis Techniques for Perfluorocarbon Tracer Derived Multizone Ventilation Rates

TED W. D'OTTAVIO*
GUNNAR I. SENUM*
RUSSELL N. DIETZ*

Several mathematical schemes for calculating ventilation flows and their associated errors using the multiple perfluorocarbon tracer (PFT) method developed at Brookhaven National Laboratory are presented and methods are suggested for their implementation on microcomputer systems. A first order error analysis method is described along with a matrix method which yields identical results but is computationally much faster. Both methods are compared to the Monte Carlo error analysis technique. The computation of an optimal condition number is suggested as a means of gauging the sensitivity of the flow solutiions.

INTRODUCTION

THE TERM building ventilation is used to describe the movement of air from one area or zone of a building to another zone and from each building zone to outdoors and vice versa. Much of the early work on building ventilation centered on measuring the total amount of outdoor air entering a building over a fixed period of time. This quantity is needed to calculate the energy necessary to heat or cool incoming air or to calculate the concentration of a pollutant generated within a building that is considered a single, well-mixed zone.

Recently, much attention has been paid to both measuring and predicting ventilation flows in buildings that are multizone in nature, i.e. buildings that consist of separate but interacting well-mixed zones. There are two primary reasons for this interest. First, tracer experiments have shown that only the simplest of residential buildings can realistically be considered single, well-mixed zones. Second, the additional interzonal flow information obtained from the multizone flow measurements are useful in answering questions related to thermal comfort and pollutant dispersion.

Over the past five years, Brookhaven National Laboratory (BNL) has developed a technique for measuring multizone ventilation in both residential and commercial buildings. This technique is an offshoot of the constant emission, steady state method of measuring air infiltration that has been around for many years. In that scheme a tracer is emitted into a building at a constant rate and its concentration is allowed to reach a steady state level. The value obtained is then converted to a flow of outdoor air into the building.

At BNL, we have extended this method to multizone ventilation measurements by using multiple perfluorocarbon tracers, one of which is emitted in each well-mixed zone of a building. Measurement of the concentrations of each tracer in all zones of the building permits the calculation of the infiltration and exfiltration air flow to each zone of the building as well as the flows between zones. The system uses passive samplers to collect the perfluorocarbon tracers and permeation tubes as tracer emitters and is, therefore, quite simple and inexpensive to implement. A detailed, experimental description of this technique is presented elsewhere [1, 2].

In this paper, we begin by examining the model behind these ventilation measurements. Although this model has been described in detail before [3, 4], we pay particular attention to the assumptions behind the model, how these assumptions relate to BNL's experimental implementation of this technique, and computational methods for calculating the ventilation flows. In addition, several methods are presented for estimating the errors in these flows that may be caused by uncertainties in the measured tracer concentrations, source emission rates and/or zonal boundaries.

STEADY STATE VENTILATION MODEL

A complete description of the ventilation characteristics of a building consists of a time-dependent characterization of the air flow rates from each well-mixed zone of the building to all other zones as well as the infiltration and exfiltration flow rates from each zone to the outdoors. In this section we describe the mathematics behind measuring these air flows using the multiple perfluorocarbon tracer gas technique developed at BNL. With slight modification, this theory can be used for other tracer gas techniques as well.

* Environmental Chemistry Division, Department of Applied Science, Brookhaven National Laboratory, Upton, NY 11973, U.S.A.

The multi-tracer, constant emission ventilation measurement technique makes the following assumptions.

(i) *A building can be divided into a set of well-mixed zones.* For this purpose, a well-mixed zone will be defined as a zone of uniform tracer gas concentration for the tracer emitted in that zone. Field measurements by BNL have shown this assumption is valid if concentration uniformity is considered to be within $\pm 10\%$. As expected, the largest deviations from the average zonal tracer concentrations occur at the zonal boundaries. Since, as we shall see, a different tracer must be used for each well-mixed zone of a building, the number of tracers available provides a practical limitation to the complexity of the building that can be studied.

(ii) *The system is at steady state over the measurement period.* With measurement periods for this technique typically in the range of 1–10 weeks, ventilation flows can and do vary significantly. However, this assumption is more robust than it might at first appear. It has been shown that typical variations in ventilation flows (50–100%) over the above time scale lead to only a 5–10% error in the average flows computed with the steady state assumption [2]. In cases where there are large, short term variations in the ventilation flows (such as frequent window openings), this technique will not provide an accurate assessment of the average ventilation flows and should be avoided.

(iii) *The emission rate of the tracers is constant.* This is usually implemented in one of two ways. The BNL implementation uses miniature permeation sources and average zonal temperatures to calculate the tracer emission rates. It has been shown that normal indoor temperature variations do not affect the accuracy of the computed air flows. A second method of producing constant tracer gas emissions is to use pressurized gas cylinders with flow control.

(iv) *Outdoor concentrations of the emitted tracers are negligible.* For the perfluorocarbon tracers used in the BNL implementation of this technique, outdoor concentrations are three orders of magnitude less than the typical 1–10 ppt (parts per trillion, volume) concentrations generated indoors. In addition, it is assumed that re-entrainment is negligible.

In the mathematics which follows, we will describe a method whereby the ventilation flows for the three zone model pictured below can be computed using multiple tracers. A general N-zone description will then conclude this section.

Let:

R_{ij} = rate of air flow from zone i to zone j ($i \neq j$; zone 0 = outdoors),

R_{ii} = sum of all air flows into or out of zone i ($i \geq 1$),

R_{00} = sum of all infiltration flows = ΣR_{0i},

C_{ij} = concentration of tracer i in zone j ($C_{i0} = 0$),

S_j = source emission rate of the tracer in zone j (constant).

Consider the three zone model shown in Fig. 1. If we emit a different tracer in each zone and measure the steady state tracer concentrations that develop for all of the tracers in all of the zones, the following tracer mass balance equations which follow can be used to measure the flows entering zone 1.

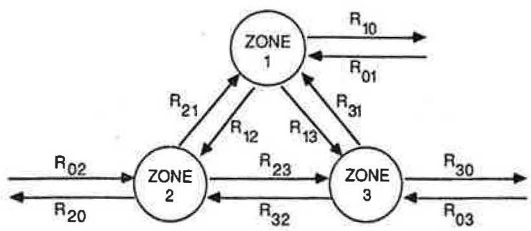

Fig. 1. Air flow schematic for a building that consists of three well-mixed zones. Zone 0 is outdoors.

$$\text{Tracer 1:}\quad R_{11}C_{11}-R_{21}C_{12}-R_{31}C_{13} = S_1. \tag{1}$$

$$\text{Tracer 2:}\quad R_{11}C_{21}-R_{21}C_{22}-R_{31}C_{23} = 0. \tag{2}$$

$$\text{Tracer 3:}\quad R_{11}C_{31}-R_{21}C_{32}-R_{31}C_{33} = 0. \tag{3}$$

$$\text{Air Flow Balance:}\quad R_{01} = R_{11}-R_{21}-R_{31}. \tag{4}$$

Since all the tracer concenrations are measured and the tracer emission rate in zone 1 is known, the tracer mass balance Equations (1–3) represent a system of three equations with three unknowns and can be solved exactly. Finally, Equation (4) is used to calculate the rate of outdoor air entering zone 1. A similar set of four equations can be set up for zone 2 and for zone 3. In this way all of the ventilation flows can be computed.

Note that once the mass balance equations are used to solve for all of the interzonal flows, air flow balance is again used to solve for the air exfiltration rate from each zone and the total building infiltration rate. For example, the following equations would be used to solve for the exfiltration rate from zone 1 and for the total infiltration rate:

$$\text{Air Flow Balance:}\quad R_{10} = R_{11}-R_{12}-R_{13} \tag{5}$$

$$R_{00} = R_{01}+R_{02}+R_{03}. \tag{6}$$

Equations (1–3), combined with the other six mass balance equations for the other two zones produce nine mass balance equations for this three zone system. In general, for N well-mixed zones, there are N^2 mass balance and $2N+1$ air flow balance equations to solve in calculating the ventilation quantities of interest. These equations can be written as follows:

$$\begin{bmatrix} C_{11} & C_{12} & \cdots & C_{1N} \\ C_{21} & C_{22} & \cdots & C_{2N} \\ \vdots & \vdots & & \vdots \\ C_{N1} & C_{N2} & \cdots & C_{NN} \end{bmatrix} \times \begin{bmatrix} R_{11} & -R_{12} & \cdots & -R_{1N} \\ -R_{21} & R_{22} & \cdots & -R_{2N} \\ \vdots & \vdots & & \vdots \\ -R_{N1} & -R_{N2} & \cdots & R_{NN} \end{bmatrix} = \begin{bmatrix} S_1 & 0 & \cdots & 0 \\ 0 & S_2 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & S_N \end{bmatrix} \tag{7}$$

$$R_{0i} = R_{ii} - \sum_{j=1}^{N} R_{ji} \tag{8}$$

$$R_{i0} = R_{ii} - \sum_{j=1}^{N} R_{ij} \tag{9}$$

$$R_{00} = \sum_{i=1}^{N} R_{0i} = \sum_{i=1}^{N} R_{i0}. \tag{10}$$

It can be shown that the tracer mass balance equations and the air flow balance equations can be combined into the following single matrix equation for the general N-zone case:

$$\begin{bmatrix} -1 & 1 & 1 & \cdots & 1 \\ 0 & C_{11} & C_{12} & \cdots & C_{1N} \\ 0 & C_{21} & C_{22} & \cdots & C_{2N} \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & C_{N1} & C_{N2} & \cdots & C_{NN} \end{bmatrix} \times \begin{bmatrix} R_{00} & R_{01} & R_{02} & \cdots & R_{0N} \\ R_{10} & R_{11} & -R_{12} & \cdots & -R_{1N} \\ R_{20} & -R_{21} & R_{22} & \cdots & -R_{2N} \\ \vdots & \vdots & \vdots & & \vdots \\ R_{N0} & -R_{N1} & -R_{N2} & \cdots & R_{NN} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ S_1 & S_1 & 0 & \cdots & 0 \\ S_2 & 0 & S_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ S_N & 0 & 0 & \cdots & S_N \end{bmatrix} \tag{11}$$

or, using boldface to denote matrices:

$$\mathbf{CR} = \mathbf{S}. \tag{12}$$

There are several methods and many pre-packaged computer programs available to solve this linear system of simultaneous equations. The three most common methods are matrix inversion, Cramer's Rule and Gaussian elimination [5]. Matrix inversion, combined with a programming language that has built in matrix operations, seems to be the easiest and fastest method for solving this equation on a microcomputer system. This method also lends itself to a relatively simple error analysis routine as will be seen in the next section. One programming language currently being used at BNL for this purpose is a new version of BASIC called True BASIC (True BASIC, Inc., Hanover, NH), which is available on both the IBM PC and Apple Macintosh line of computers. IBM BASICA combined with an add on set of matrix commands contained in the Matrix 100 package (Stanford Business Software, Inc., Palo Alto, CA) works well also.

ERROR ANALYSIS METHODS

Input variable errors

Several methods are available for estimating the errors in the computed ventilation flows. These methods are based on estimates of the precision of the measured tracer concentrations and source emission rates. Before we delve into methods for estimating errors in the computed flows, we would briefly like to describe how we have attempted to estimate the errors in the input tracer concentration and source rate values.

As mentioned previously, the BNL perfluorocarbon technique uses permeation tubes as tracer emission sources. At a known temperature, the permeation rates of these tubes are well known since the sources are gravimetrically calibrated at 25°C and the temperature dependence is well known [2]. However, the emission rate of these tubes is exponentially dependent on temperature (a 3°C change in temperature leads to a 15% change in the permeation rate) and uncertainties in estimating average indoor temperatures leads to the major source of error in estimating the tracer permeation rates in a building. Unless temperature measurements are very precise, we estimate that average indoor temperature can be measured within ± 2°C leading to an estimated error in the tracer source rates of about $\pm 10\%$.

Errors in the zonal tracer concentrations come from inaccuracies in measuring the tracer concentration at a given location and from differences between tracer samples taken at various locations within a zone that is considered well-mixed. Side by side samplers have shown that tracer concentrations measured at a given location do not differ by more than 2% [2]. However, depending on the building and the way the sources and samplers were placed, multiple samplers in a given zone can differ significantly. This is the major cause of uncertainty in the zonal tracer concentrations. We use the standard deviation of these multiple measurements as an estimate of the error in the tracer concentrations. If only one sampler is used, we estimate this error to be $\pm 10\%$.

For all of the error analysis methods which follow, we assume that a random sampling of source emission rate and tracer concentration measurements would produce a Gaussian distribution with mean given by the average of the measured values and standard deviation given by the estimated error.

First order error analysis

The first order error analysis procedure is the most commonly used error propagation procedure and much has been written about it [6]. First order analysis is based on the Taylor series expansion, which states that if $x = f(u)$, then the change in x (Δx) produced by a change in u (Δu) is given by:

$$\Delta x = \frac{\partial x}{\partial u}\Delta u + \frac{\partial^2 x}{\partial u^2}(\Delta u^2/2!) + \frac{\partial^3 x}{\partial u^3}(\Delta u^3/3!) + \cdots.$$

If we assume that the first term in the above summation is dominant and extend to multivariate form, it can be shown that, for a general function of the form $x = f(u, v, \ldots)$, the variance in x, equivalent to the square of the standard deviation, is given approximately by:

$$s_x^2 = \left(\frac{\partial x}{\partial u}\right)^2 s_u^2 + \left(\frac{\partial x}{\partial v}\right)^2 s_v^2 + \cdots. \tag{13}$$

The above equation results from the Taylor series expansion of x about its mean value and truncation of the

190 + 191 ontbreken

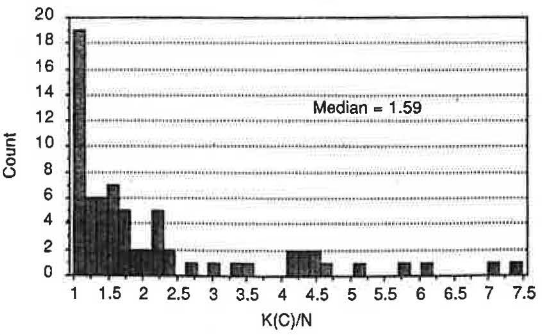

Fig. 3. Frequency distribution for values of the optimal condition number divided by the number of zones using tracer concentration measurements made in 60 two and three zone homes.

(i.e. they are well-mixed), then the determinant of the concentration matrix will approach zero, the condition number will approach infinity and the errors on the computed flows will approach infinity.

In addition to its usefulness in measuring the sensitivity of the mass balance equations to changes in the input parameters, the condition number can also be used to estimate average flow errors. Using a set of 60 two and three zone residential homes, we explored various equations that could be used to estimate the effects of the condition number, the source rate errors and tracer concentration errors on the average computed flow errors. The equation which best fit this limited set of data is shown below:

$$\frac{\|\Delta \mathbf{R}\|}{\|\mathbf{R}\|} = \frac{\|\Delta \mathbf{S}\|}{\|\mathbf{S}\|} + 0.67\frac{K(\mathbf{C})}{N}\frac{\|\Delta \mathbf{C}\|}{\|\mathbf{C}\|}. \tag{17}$$

Figure 4 shows a comparison of the average flow errors computed with Equation (17) and the average errors computed with the first order error analysis. The agreement is quite good over a wide range of condition numbers (1.00–58.01) and flow errors (10–651%). Source rate errors were set at 10% while average concentration errors ranged from 2–30%. Note, however, that this agreement did not hold in several cases where average concentration errors were around 50% as might be expected since both error analysis schemes assume that the concentration errors are low compared with the concentrations.

Walker [10] has previously applied the condition

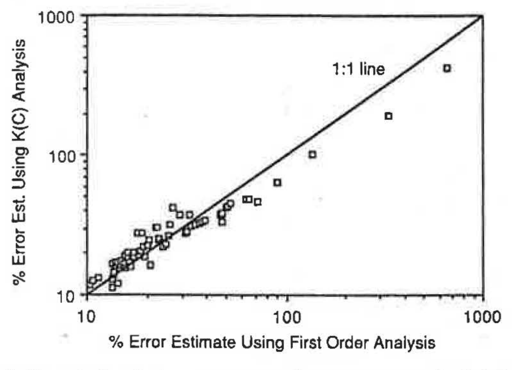

Fig. 4. Correlation between average flow errors as calculated by a first order error analysis and by an error analysis using the optimal condition number.

number concept to the interpretation of average errors in multizone infiltration experiments. However, Walker used an earlier definition of the condition number [9] and consequently his analysis was not as successful as the use of the optimal condition number, which is scale invariant [7, 8].

As can be seen from the optimal condition number analyses, the ventilation rate errors will be magnified when the concentration matrix is ill-conditioned, which results when at least two zones are well-coupled, i.e., there is a relatively large interzonal flow between these zones compared to the total ventilation flow through these zones. This magnification of ventilation errors can be reduced by condensing the well-coupled zones into a single zone. In many instances, what may physically appear to be distinct zones are, in fact, well-coupled and behave as single zones. This elimination of well-coupled zones into single zones reduces ventilation rate errors, but with a consequent loss of being able to determine the interzonal rates between these well-coupled zones. As a result, if a determination of the interzonal flows between well-coupled zones is needed, they will have relatively large errors associated with them compared to the errors in the input concentrations and source rates.

Monte Carlo error analysis

All of the error analysis schemes mentioned above make the assumptions listed in the first order error analysis section, i.e. the input variables are uncorrelated, have symmetric probability distributions and have negligible high order Taylor series terms at their measured values. The Monte Carlo error analysis method makes none of these assumptions and can, therefore, be used to check the validity of the results from the other error analysis methods.

With this method, probability distributions are assigned to each of the input variables and a value for each is randomly selected based on these probabilities. These values are inserted into the model equations and a set of flows are computed. After this is repeated a large number of times, a distribution for each flow is obtained which accurately indicates the uncertainty in its value, irregardless of the magnitude of the uncertainties in the input variables or their particular distributions.

We compared the results of the Monte Carlo error analysis using 1000 trials with the results obtained with the first order analysis for three homes which span a range of tracer concentration errors and optimal condition numbers. House A has low estimated concentration errors and a low condition number, house B has high concentration errors and a low condition number and house C has low concentration errors and a high condition number. The magnitude of these values can be seen in Table 1 along with flow results and errors computed with both methods. Gaussian distributions are assumed for the input variables.

For house A, the agreement between the Monte Carlo and first order error analysis methods was excellent for both the flow averages and their standard deviations. However, the agreement was poor for both houses B and C. Figures 5 and 6 show the distributions obtained for two of the flows using the Monte Carlo analysis on the three homes. For house A the distributions are Guassian-

Table 1. Comparison of the First Order and Monte Carlo error analysis schemes for three test homes. House A has a low optimal condition number ($K(\mathrm{C})/N$) and low tracer concentration errors ($\|\Delta C\|/\|C\|$). House B has a low $K(\mathrm{C})/N$ and a high ($\|\Delta C\|/\|C\|$). House C has a high $K(\mathrm{C})N$ and a low ($\|\Delta C\|/\|C\|$)

				First Order Error Analysis				Monte Carlo Error Analysis			
House	$\frac{\|\Delta C\|}{\|C\|}$	$\frac{\|\Delta R\|}{\|R\|}$	$\frac{K(\mathrm{C})}{N}$	R_{12}	ΔR_{12}	R_{00}	ΔR_{00}	R_{12}	ΔR_{12}	R_{00}	ΔR_{00}
A	0.077	0.162	1.40	132.6	43.4	732.1	59.5	136.1	44.4	738.6	63.1
B	0.410	0.161	1.47	192.8	129.3	1547.5	128.2	241.2	196.6*	1550.8	148.8†
C	0.081	0.481	5.14	587.4	285.6	381.2	46.7	703.6	416.6‡	376.9	68.9§

* Excludes 17 data points > 130 with average = 4148 and 15 data points < −200 with average = −10,617. With these points, the average = 184.6 and the standard deviation = 3578.6.

† Excludes 2 data points > 2200 with average = 5559 and 2 data points < 1000 with average = 350. With these points, the average = 1556.4 and the standard deviation = 280.8.

‡ Excludes 26 data points > 3000 with average = 17,565 and 28 data points < 0 with average = −10,277. With these points, the average = 943.7 and the standard deviation = 7063.5.

§ Excludes 6 data points > 800 with average = 2086 and 6 data points < 0 with average = −3220. With these points, the average = 365.6 and the standard deviation = 460.4.

looking with no extreme outliers. For houses B and C, the distributions are asymmetric and there are several extreme outliers (see Table 1).

Notice that the disagreement between the two error analysis schemes and the skewness of the distribution curves is particularly bad for the interzonal (R_{12}) flow and error computations while more moderate for the overall infiltration (R_{00}) results. This is a pattern that we have repeatedly noticed. The stability of the solution for the overall infiltration flow is much greater than that for the solutions of the interzonal flows. This intuitively makes sense although it is difficult to justify mathematically.

These results and others that we have obtained have showed that the first order, matrix and/or condition number error analysis schemes must be used with care in order to obtain meaningful results. In general, we have found that greater than a 25% error in the tracer concentrations and/or a value for $K(\mathrm{C})/N > 2N^{1/2}$ can cause serious problems with these methods. Although computationally intensive, the Monte Carlo error method can be used to give more realistic error estimates in these cases.

SUMMARY

In this paper we have presented several mathematical schemes for calculating ventilation flows and their associated errors using the multitracer, constant emission method for measuring building ventilation developed at Brookhaven National Laboratory. This method can be implemented by emitting a different tracer into each well-mixed zone of a building at a known and constant emission rate and measuring the resulting steady state tracer

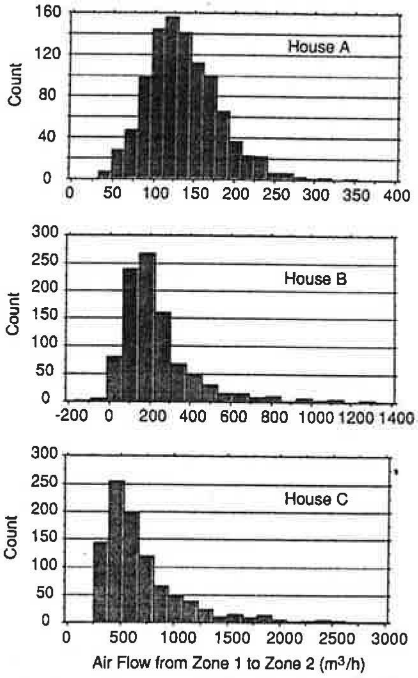

Fig. 5. Distribution of interzonal flows for three test homes using a Monte Carlo simulation with 1000 trials. Note deleted points in Table 1.

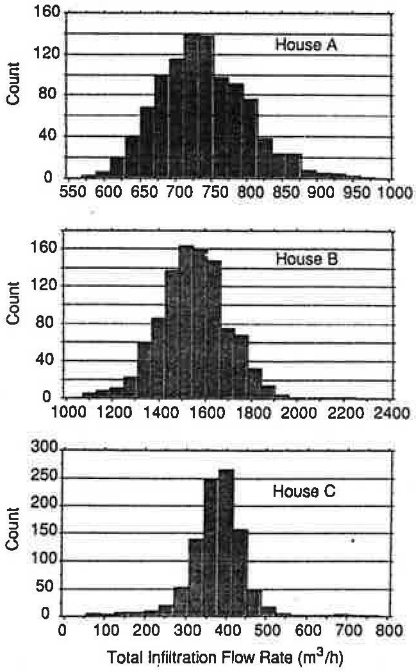

Fig. 6. Distribution of infiltration flow rates for three test homes using a Monte Carlo simulation with 1000 trials. Note deleted points in Table 1.

concentrations that exist in each zone. The assumptions associated with this technique are discussed.

It is shown that for a building with N well-mixed zones, N^2 mass balance equations and $2N+1$ flow balance equations can be generated to solve for all of the infiltration, exfiltration and interzonal flows. The above equations have been incorporated into a single matrix equation which can be used to easily solve for the ventilation flows.

Several error analysis methods are proposed for estimating the errors in these computed flows. These errors are based on errors in the model inputs (the measured tracer concentrations and emission rates), which primarily result from zonal concentration variations based on multiple samplers and errors in estimating the average temperature of the permeation sources used to emit the tracers.

A first order error analysis scheme, based on a Taylor series expansion of the flow solutions around their average values, is described along with a matrix method which yields identical results but is computationally much faster. Methods are suggested for implementing the matrix method on a microcomputer system.

A third method for estimating average flow errors, based on the computation of an optimal condition number is also described. The optimal condition number can be used as a guide to estimating the sensitivity of the flow solutions to small changes in the input variables. One example which leads to a high value for the condition number and, therefore, high flow errors is when zones that are considered separate are actually well-mixed with each other. The condition number can also be used, along with the average errors in the tracer concentrations and emission rates, to estimate the average error in the computed flows. An equation is developed for this purpose.

Each of the above error analysis methods assume that the relative errors in the input variables are small and that the flow solutions are not very nonlinear. Since either or both of these assumptions may not be true in all practical cases, we compared the results from the above error analysis schemes with a Monte Carlo error analysis which makes neither of these assumptions. The results of this comparison indicate that the assumptions behind the first order, matrix and condition number error analysis methods begin to break down when the concentration errors exceed 25% or when $K(\mathbf{C})/N > 2N^{1/2}$ where $K(\mathbf{C})$ is the optimal condition number and N is the number of well-mixed zones.

Acknowledgement—This research was performed under the auspices of the United States Department of Energy under Contract No. DE-AC02-76CH00016.

REFERENCES

1. R. N. Dietz and E. A. Cote, Air infiltration measurements in a home using a convenient perfluorocarbon tracer technique, *Environ. Int.* **8**, 419–433 (1982).
2. R. N. Dietz, R. W. Goodrich, E. A. Cote and R. F. Wieser, Detailed description and performance of a passive perfluorocarbon tracer system for building ventilation and air exchange measurements, *Measured Air Leakage of Buildings*, ASTM STP 904, p. 203–64, American Society for Testing and Materials, Philadelphia (1986).
3. F. W. Sinden, Multi-chamber theory of air infiltration, *Bldg Environ.* **13**, 21–28 (1978).
4. M. Sandberg, The muli-chamber theory reconsidered from the viewpoint of air quality studies, *Bldg Environ.* **19**, 221–233 (1984).
5. V. N. Faddeeva, *Computational Methods of Linear Algebra*, Dover, New York (1959).
6. P. R. Bevington, *Data Reduction and Error Analysis for the Physical Sciences*, McGraw-Hill, New York (1969).
7. F. L. Bauer, Optimally scaled matrices, *Numerische Mathematik* **5**, 73–87 (1963).
8. C. McCarthy and G. Strang, Optimal conditioning of matrices, *SIAM J. Numer. Anal.* **10**, 370–388 (1973).
9. A. M. Turing, Rounding-off errors in matrix processes, *Q. J. Mech. Appl. Math.* **1**, 287–308 (1948).
10. R. R. Walker, Interpretation and error analysis of multi-tracer gas measurements to determine air movements in a house, Sixth Air Infiltration Center Conference, paper S.3, (1985).