A METHOD FOR IMPROVED MEASUREMENT OF GAS CONCENTRATION HISTORIES IN RAPIDLY DEVELOPING FIRES

By

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ABSTRACT

A method is described for improving the transient gas concentration measurement in a relatively fast-developing fire or in any changing environment with a characteristic transient time that is comparable to the response time of the sampling system (including analyzer). Under such conditions, the measurements can be significantly altered in both time and magnitude and, hence, be of limited usefulness. The method utilizes the result of a simple laboratory test - the response of the measuring system to a step input - to determine the sampled concentration history from the analyzer record.

INTRODUCTION

In many fire research projects, the concentration of various gas species is of prime importance, and, in some cases, a continuous time record of this quantity is desired. This is achievable with the use of continuous-flow gas analyzers. In most cases, to ensure accuracy and instrument protection, it is necessary to aspirate the gas entering the sampling port through a system of condensers, filters and desiccators before it passes through the analyzer. If the flow through this system were ideal plug flow, the measured output would represent the input to the sampling port accurately although shifted in time by the transit time through the system. However, as a result of viscosity effects, diffusion, turbulent mixing and analyzer response, the actual transient record from the analyzer is delayed and distorted with respect to time. For a steady-state experiment, this presents no problem, but for a transient measurement, the output of the analyzer can be significantly different from the input to the sampling port. This paper describes a method of improving the accuracy of such measurements, both in time and magnitude.

It is well known that, for a linear, time-varying system involving a single dependent variable, an input/output relationship can be obtained by solving the ordinary differential equation that describes the system. This approach is quite useful in practice when the differential equation is known, e.g., in electrical circuit theory.

In those cases where the differential equation of an experimental system is not known, a simple laboratory test - the system response to a step input - can be used to determine the input/output relationship. This has been used successfully 1) in reactor theory to analyze flow through packed beds via a residence time distribution (Levenspiel, 1962) and 2) in control theory via an open loop transfer function (Harriott 1964). The response to the step input is utilized to generate the governing differential equation, or, equivalently, the open loop transfer function. With these mathematical approximations, one can predict the system output for any input of interest.

Most present-day applications are concerned primarily with determining the output for a given input or determining any input that yields a prespecified output. In the present application, in which the input corresponds to the actual gas concentration at the sampling port and the output corresponds to the analyzer record, the objective is to determine the input that causes the measured output.

GAS CONCENTRATION MEASUREMENTS IN FIRE TESTS

Fire tests can range from small, well controlled laboratory experiments to very complex, full-scale investigations. In a recent study of vented enclosure fires (Croce 1974), the enclosure environments, including the concentration of various gas species, were compared in large and small scale. Wood cribs that were appropriately scaled with the enclosure size were used as the fuel bed. For the small laboratory size enclosure with ample ventilation, the quasi-steady burning duration was on the order of 1-2 min. A magnetic susceptibility oxygen analyzer can have an inherent rise time* (t_r) of 10-40 sec. When connected to a series of condensers, filters, dessicators,

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*Time required to respond from 10 percent to 90 percent of a step concentration input.

etc., the system delay time* (t_d) can become one minute or more. These times are depicted in Figure 1 (in which c is the instantaneous concentration and C_o, the constant input concentration). If such a system is used to monitor the oxygen environment of a laboratory crib fire, the resulting concentration record is of very limited usefulness in determining either the concentration at any instant of time during the burn, or the average concentration throughout the burn interval. This is illustrated in Figure 2.

To improve the accuracy of this measurement, assuming the analyzer to be sufficiently linear, the typically exponential response to the step input, i.e., the output curve of Figure 1, is fitted to an exponential function with the desired degree of accuracy (±2 percent of maximum value is not unreasonable); several methods are available, the easiest of which, especially for functions involving more than one exponential term, is a graphical method that is outlined by Harriott (1964). The function is chosen such that it represents a series of linear, non-interacting, exponentially-responding elements (one or more, as needed) that approximates the actual gas concentration measuring system. The graphical method yields the lag time (t_L) and time constant (t_c) of the various elements** of the equivalent analytical system, quantities which are necessary for the development of this method.

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* Time required to respond to 90 percent of a step concentration input.

** "Lag time" is the duration of the zero-response portion of the output curve of Figure 1; the "time constant" of a single, linear element is the time required to respond to 63 percent of a constant input value.

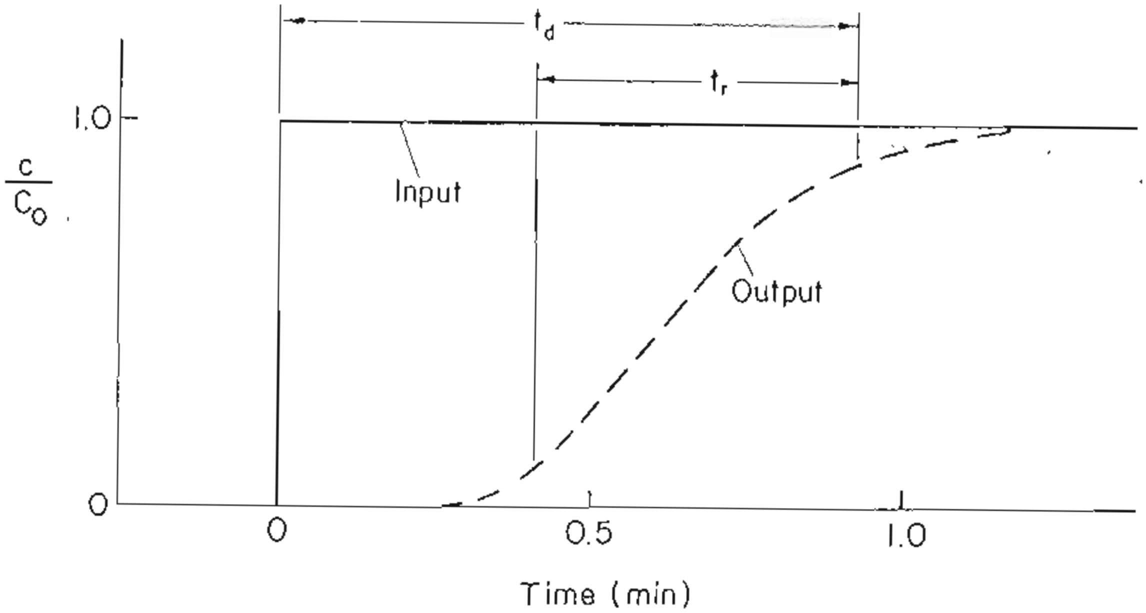

FIGURE 1. GAS CONCENTRATION SYSTEM RESPONSE TO STEP INPUT

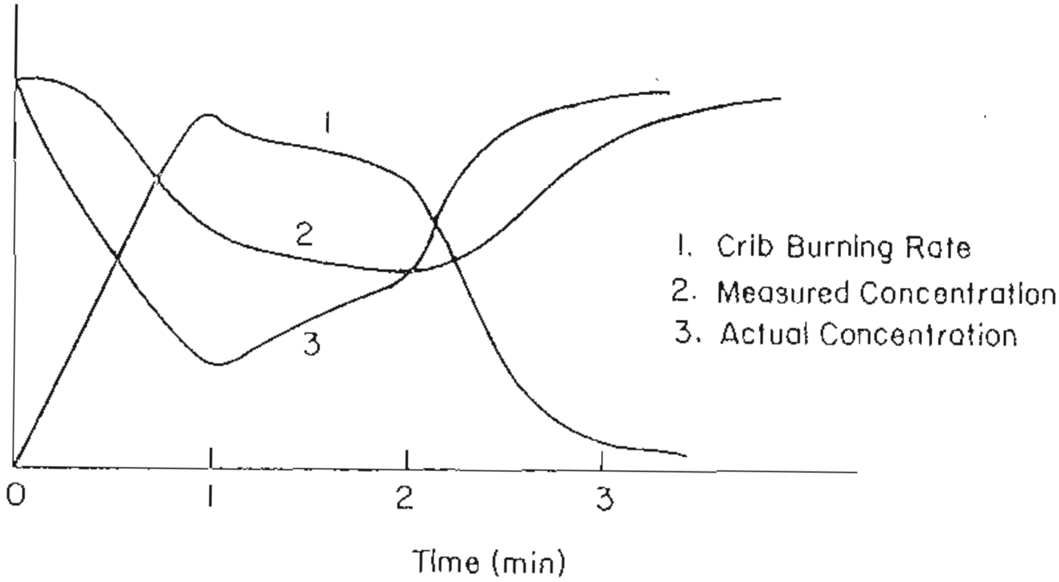

FIGURE 2. ERROR IN GAS CONCENTRATION HISTORY USING A RELATIVELY SLOW-RESPONDING ANALYZING SYSTEM

Physically, the chosen exponential function can be interpreted as representing the entire, real, constant flow system as a series of well-stirred tanks (linear elements), each with its own characteristic hold-up time* (time constant); the number of tanks and their appropriate time constants are determined, through the graphical curve-fitting method, such that the overall effect of viscosity, diffusion and turbulence in all of the components of the total system is adequately modeled.

Once the response to the step input has been curve-fitted satisfactorily, several techniques may be used to obtain the input (the true gas concentration history at the gas sampling port) corresponding to the measured system output (the time record of gas concentration as generated by the analyzer). Three of these techniques were investigated - the differential-equation technique, the inversion integral technique, and the transfer function technique. These techniques will be discussed briefly here and presented in detail with the use of an example in the Appendix; since the recorded output for burn tests is usually not easily expressed analytically, the various techniques are treated numerically.

Differential Equation Technique

For this approach, one must determine the linear differential equation which is satisfied by the curve-fitted approximating function. For simple exponential functions, the desired differential equation is easily found by working backwards from the characteristic equation of the differential equation (Hildebrand 1962). The differential equation will involve the constants t_L and t_c, a forcing function (a constant for the step response) and necessary

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*Tank volume divided by volumetric flow rate initial and lag time conditions. If the actual forcing function for the test burn (the sampling port concentration is substituted for the step forcing function, the result is a differential equation that describes the measurement for all time (subject to initial and lag time conditions) during the test. This equation can, therefore, be applied at any instant of time to determine the only unknown - the concentration at the sampling port - in terms of t_L, t_C, and derivatives of the recorded output curves (see the Appendix).

Inversion Integral Technique

In this approach, the measured output is formulated as the integrated summation of step responses corresponding to the infinitesimal input step changes over the desired time interval. The resulting integral is then inverted to obtain the input (sampling port) concentration history. For sufficiently simple step response functions, the integral can be inverted analytically, but in most practical situations, the inversion must be treated numerically (Bellman et al. 1966). The present treatment is shown in the Appendix.

Transfer Function Technique

In control theory, the open loop transfer function of a linear input/output (I/O) system can be found using Laplace transforms. Basically, the transfer function is the ratio of the transformed output to the transformed input and remains invariant in the Laplace transform variable domain (Harriott, 1964). Hence, if it is known for one I/O condition, it is known for all I/O conditions. The transfer function for the gas concentration measuring system can be found for the step input case using the fitted exponential function for the output. Thus, to obtain the true gas concentration history, one need only divide the Laplace transform of the measured output by the transfer function and determine the inverse Laplace transform of the quotient.

The result using any of these techniques is a calculated value of the input to the gas concentration measuring system. Before any of the techniques can be used reliably, however, it must be verified; the results of an independent laboratory test are described in the next section.

RESULTS

The various techniques were tested by sampling a series of coupled CO_2 and O_2 concentration steps of arbitrary, but controlled, magnitude and duration, and comparing the known input to the input determined from the output (analyzer record). The apparatus is shown in Figure 3; a steady-state calibration of the rotameter was performed beforehand. The system allowed a CO_2 range of 0-25 percent (by volume) coupled with a 21-14 percent variation of O_2. The arbitrary concentration steps were obtained by opening or closing the control valve rapidly (2-3 sec). The total test duration was 9 min. The results for O_2 and CO_2 are presented in Figures 4 and 5, respectively, and include the measured input, the measured analyzer output and calculated input.* Immediately obvious in the figures is how misleading the recorded output can be when

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*For these tests, t_L = 21.3 sec and t_c = 14.4 sec for O_2 and t_L = 21.3 sec and t_c = 1.5 sec for CO_2. The analyzers used were a Beckman Model F-3 (magnetic susceptibility) for O_2 and a Beckman Model 315A (infrared absorption)for CO_2.

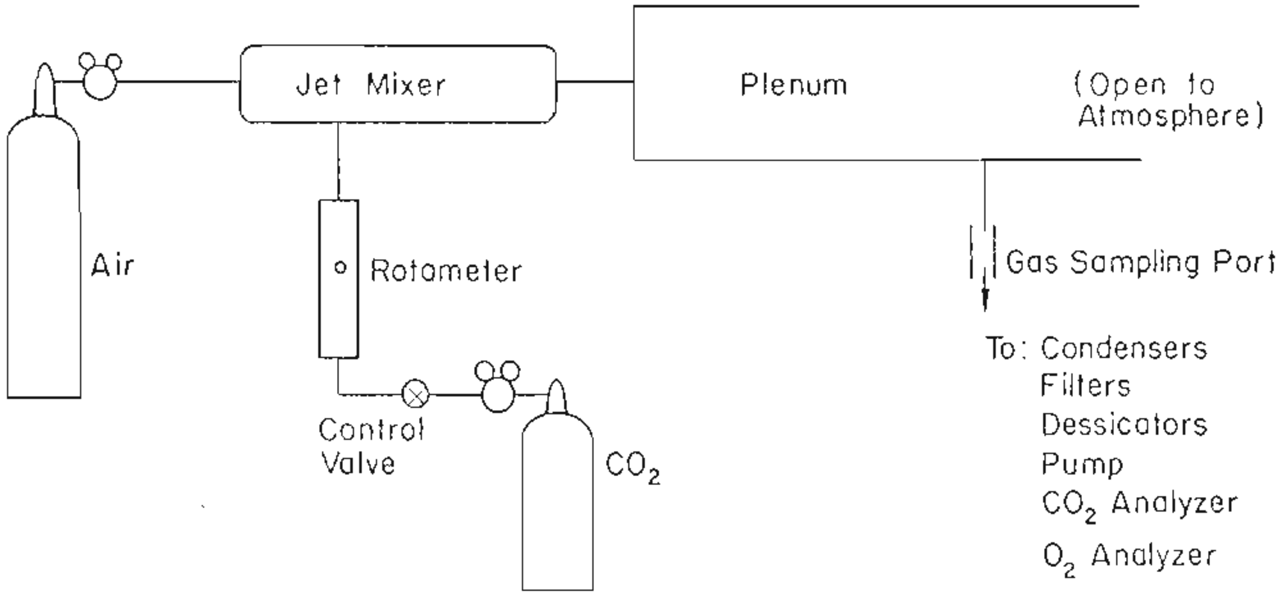

FIGURE 3. LABORATORY SETUP FOR TESTING METHOD OF IMPROVING GAS CONCENTRATION MEASUREMENT

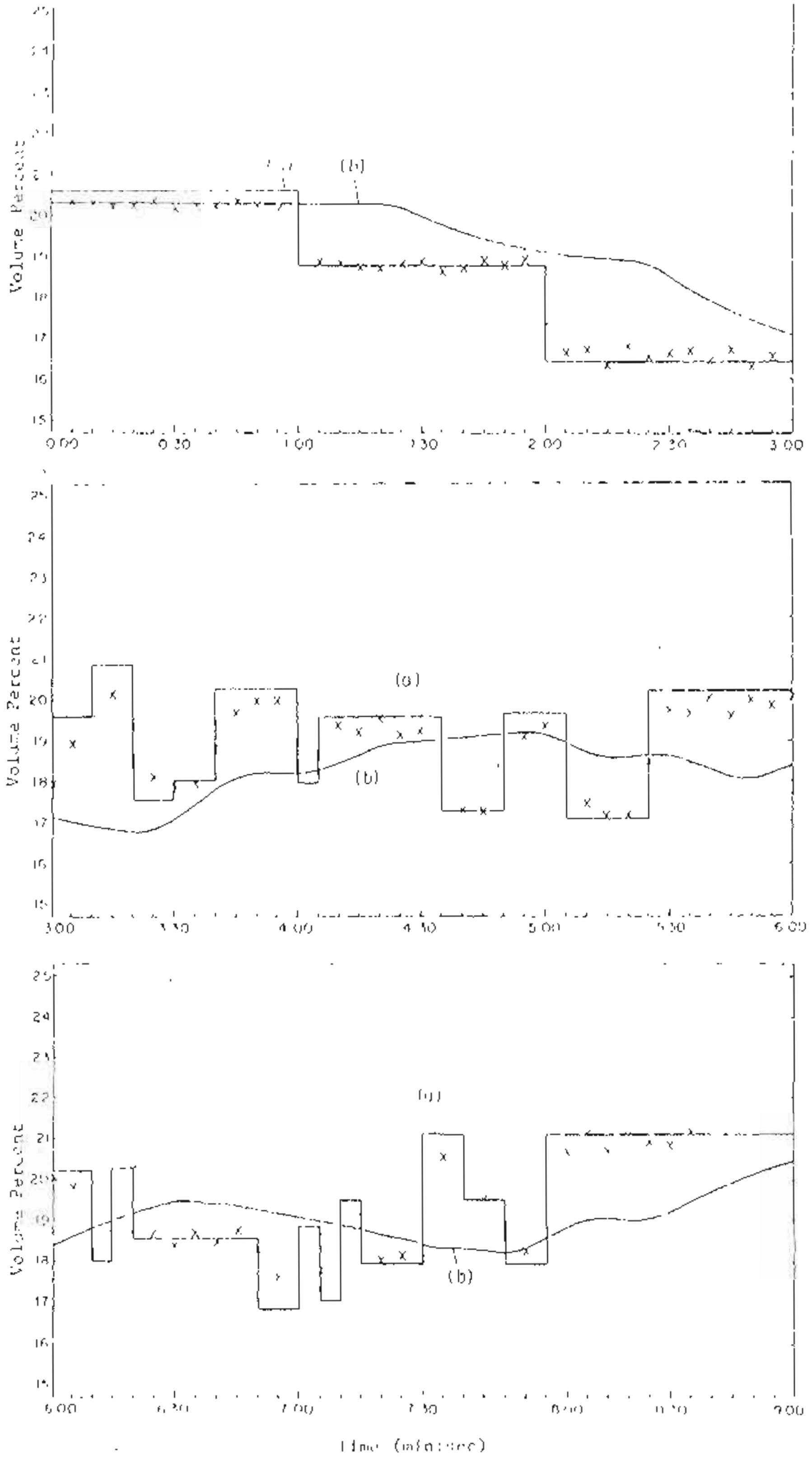

FIGURE 4. TEST RESULTS FOR OXYGEN: (a) MEASURED INPUT; (b) MEASURED OUTPUT; X - CALCULATED INPUTS

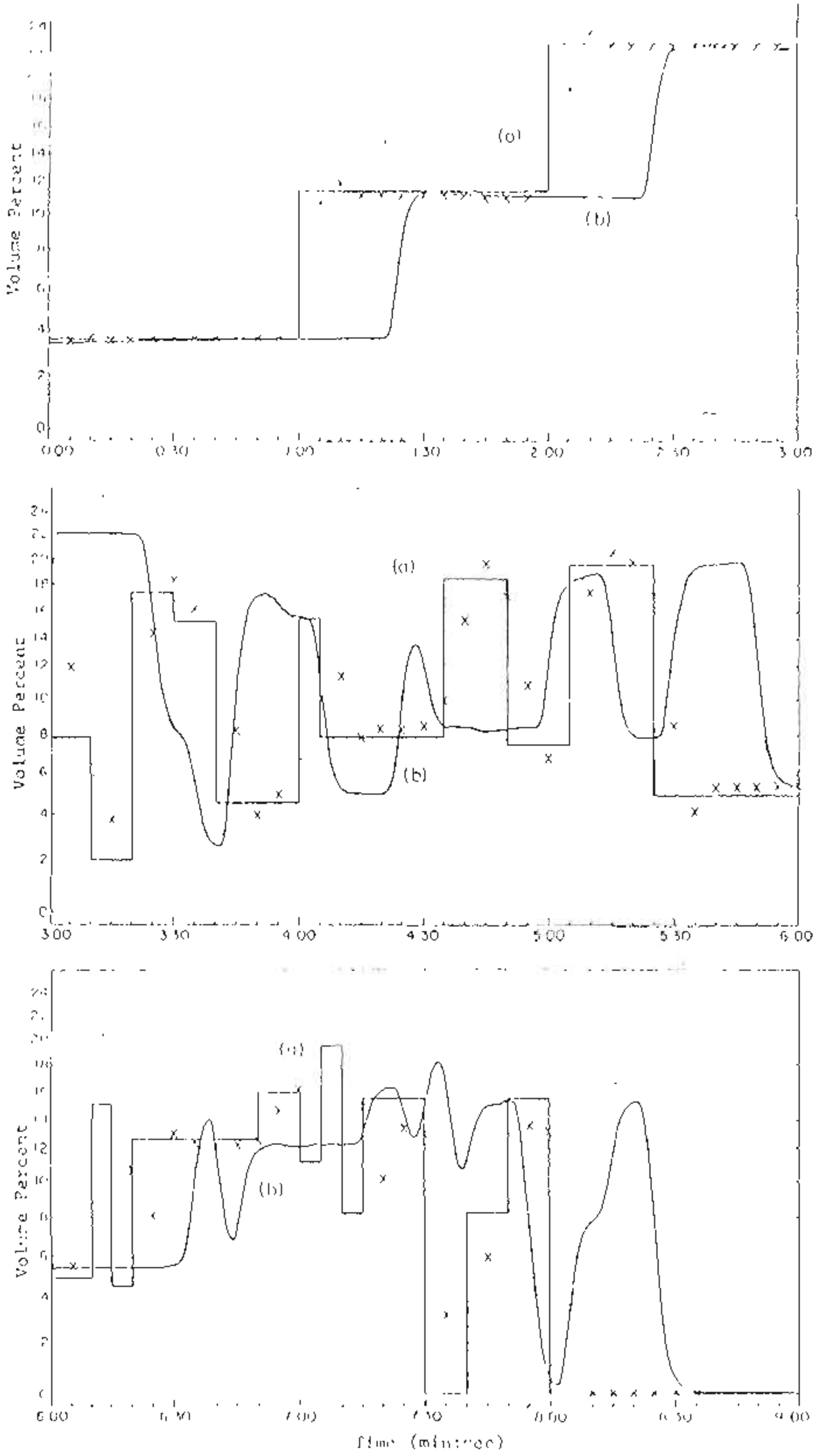

FIGURE 5. TEST RESULTS FOR CARBON DIOXIDE: (a) MEASURED INPUT; (b) MEASURED OUTPUT; X - CALCULATED INPUT

compared to the measured input (especially for O_2). The figures also show that the calculated inputs provide significantly better measures of the true inputs than do the measured outputs.

The calculated inputs shown in Figures 4 and 5 are the results of applying the differential equation technique to the measured output curves. The results of the inversion integral technique were essentially identical, although the differential equation technique responded slightly faster to the rapid step changes. A comparison of the results of these two techniques is shown in Figure 6 for the 6-9 min O_2 test interval.

The transfer function technique did not perform so well; an instability in the Laplace transform inversion computation, a not uncommon problem (Bellman et al. 1966), led to results which were not useful; some calculated points by this technique are also shown in Figure 6. Since both of the other techniques yielded very satisfactory results and were considerably less complex to formulate, no further work was done to improve or refine the transfer function technique.

DISCUSSION

This method for improving the time record of a gas species concentration measurement is helpful whenever the analyzing system response to a step input is significantly spread out over a time that is comparable to or greater than an important characteristic experiment time (t_{ch}), i.e., whenever $t_r \sim t_{ch}$ or $t_r > t_{ch}$ (see curve (b) of Figure 7). The analyzing system must also be sufficiently linear. The method is not advantageous to use when the rise time

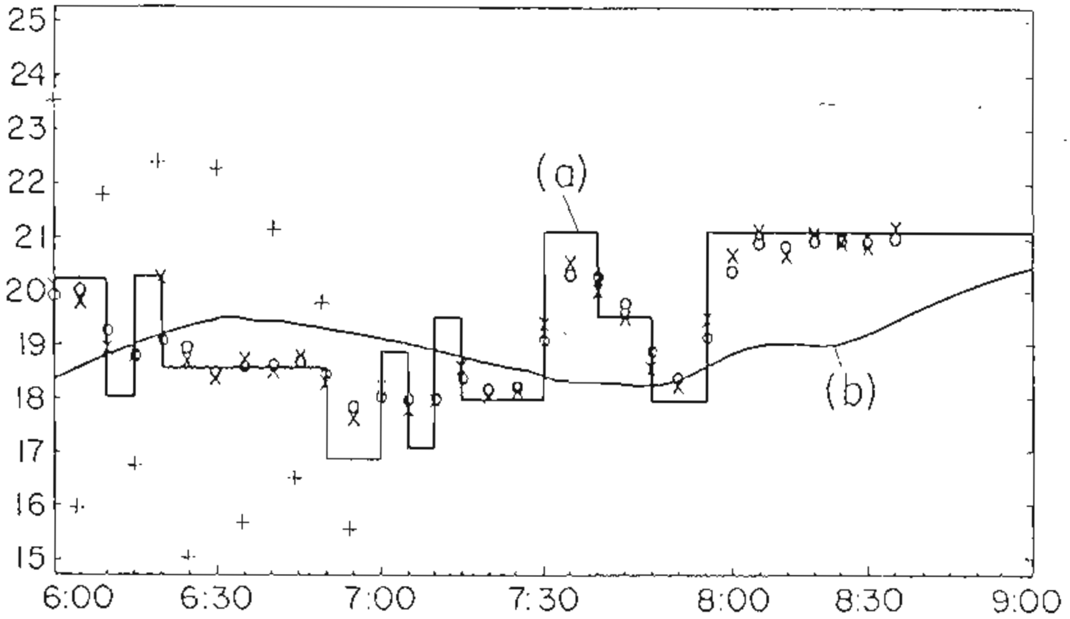

FIGURE 6. COMPARISON OF RESULTS BY ALL THREE TECHNIQUES FOR THE 6-9 MINUTE OXYGEN TEST INTERVAL. (a) MEASURED INPUT; (b) MEASURED OUTPUT; CALCULATED INPUT BY X - DIFFERENTIAL EQUATION TECHNIQUE, o - INVERSION INTEGRAL TECHNIQUE, + - TRANSFER FUNCTION TECHNIQUE

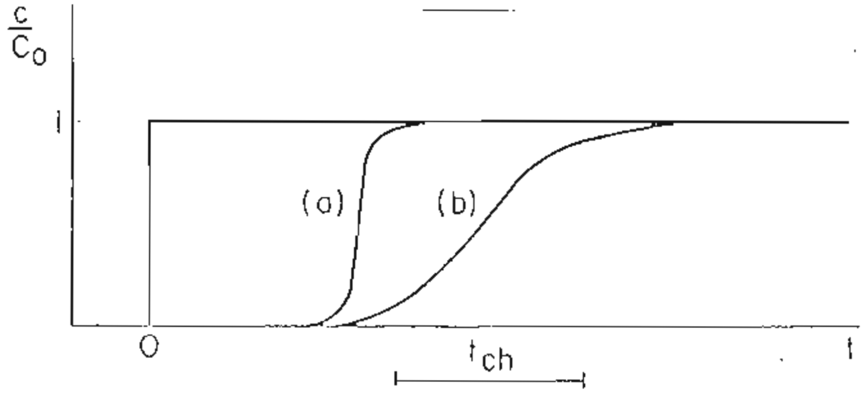

FIGURE 7. COMPARISON OF RELATIVELY (a) FAST- AND (b) SLOW-RESPONDING SYSTEMS WITH CHARACTERISTIC EXPERIMENT TIME. PRESENT METHOD IS USEFUL WHEN CURVE (b) IS OBTAINED

is small compared to the characteristic experiment time, i.e., $t_r << t_{ch}$ (curve (a) in Figure 7); in this case, a mere time shift equal to the delay time, t_d, is adequate (see, for example, Figure 5).

Both the differential equation technique and the inversion integral technique yielded satisfactory results. The former is very simple and straightforward to use and can be applied locally in time, which is a desirable feature for numerical calculations; however, this technique is susceptible to inaccuracies associated with numerical differentiation. The latter technique, on the other hand, has the advantage of being less sensitive to local irregularities since the calculated input value at a particular instant of time depends on the entire previous data history. Both of these techniques have been used successfully in the data reduction by computer of laboratory and large-scale fire tests.

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REFERENCES

BELLMAN, R., Kalaba, R.E. and Lockett, J.A., Numerical Inversion of the Laplace Transform, American Elsevier, New York, 1966.

CROCE, P.A., "Modeling of Vented Enclosure Fires," Eastern Section Meeting of the Combustion Institute, Applied Physics Laboratory, Johns Hopkins University, November 1974.

HARRIOTT, P., Process Control, McGraw-Hill, New York, 1964.

HILDEBRAND, F.B., Advanced Calculus for Applications, Prentice Hall, Englewood Cliffs, N. J., 1962.

LEVENSPIEL, O., Chemical Reaction Engineering, Wiley, New York, 1962.

APPENDIX

DIFFERENTIAL EQUATION TECHNIQUE

Let $x(t)$ be the unknown but desired input to the gas sampling port and $y(t)$ the recorded output of the analyzer; $x_s(t)$ and $y_s(t)$ are the corresponding quantities for the step input and response. For each gas species concentration measuring system in our laboratory setup, a normalized step input, i.e., $c/C_o = x_s(t) = 1.0$ for $t>0$, yielded an output that was closely approximated by

$$y_s(t) = \begin{cases} 0\ , \text{ for } t<t_L, \\ 1 - [1 + (t-t_L)/t_c]\ \exp[-(t-t_L)/tc], \text{ for } t \geq t_L, \end{cases} \tag{1}$$

where t is time and t_L and tc are, respectively, the lag time and time constant (different set for each gas species measuring system). This function represents a series of two linear elements, each with the time constant t_c.

If we let $t^* = t-t_L$, we have

$$y_s(t^*) = 1 - [1 + t^*/t_c]\ \exp[-t^*/t_c], \text{ for } t^* > 0. \tag{2}$$

This function satisfies the following differential equation, which may be interpreted as a description of the measurement:

$$t_c^{\ 2}\ \frac{d^2 y_s(t^*)}{dt^{*2}} + 2t_c\ \frac{dy_s(t^*)}{dt^*} + y_s(t^*) = 1, \text{ for } t^* \geq 0. \tag{3}$$

Note that the left hand side describes the system while the right hand side is the forcing or driving function, $x_s(t^*)$. If the system remains unchanged when the actual measurement is made, the forcing function is $x(t^*)$ and we have

$$t_c^2 \frac{d^2y(t^*)}{dt^{*2}} + 2t_c \frac{dy(t^*)}{dt^*} + y(t^*) = x(t^*), \text{ for } t^* > 0. \qquad (4)$$

In real output time, this is

$$t_c^2 \frac{d^2y(t)}{dt^2} + 2t_c \frac{dy(t)}{dt} + y(t) = x(t-t_L), \text{ for } t \geq t_L, \qquad (5)$$

and in real input time,

$$x(t) = t_c^2 \frac{d^2y(t+t_L)}{dt^2} + 2t_c \frac{dy(t+t_L)}{dt} + y(t+t_L), \text{ for } t \geq 0. \qquad (6)$$

Thus, in a numerical scheme, the actual input at time t is determined by the constant t_c and the first and second derivatives of the measured output, y, at the time $t+t_L$.

INVERSION INTEGRAL TECHNIQUE

With the same notation, assume x(t) to be a series of steps, as in Figure 8b, each of which gives rise to a response function of the type measured, $y_s(t)$, as in Figure 8a. For infinitesimal steps, the measured output, y(t), can be expressed as an integrated summation of corresponding step responses, i.e.,

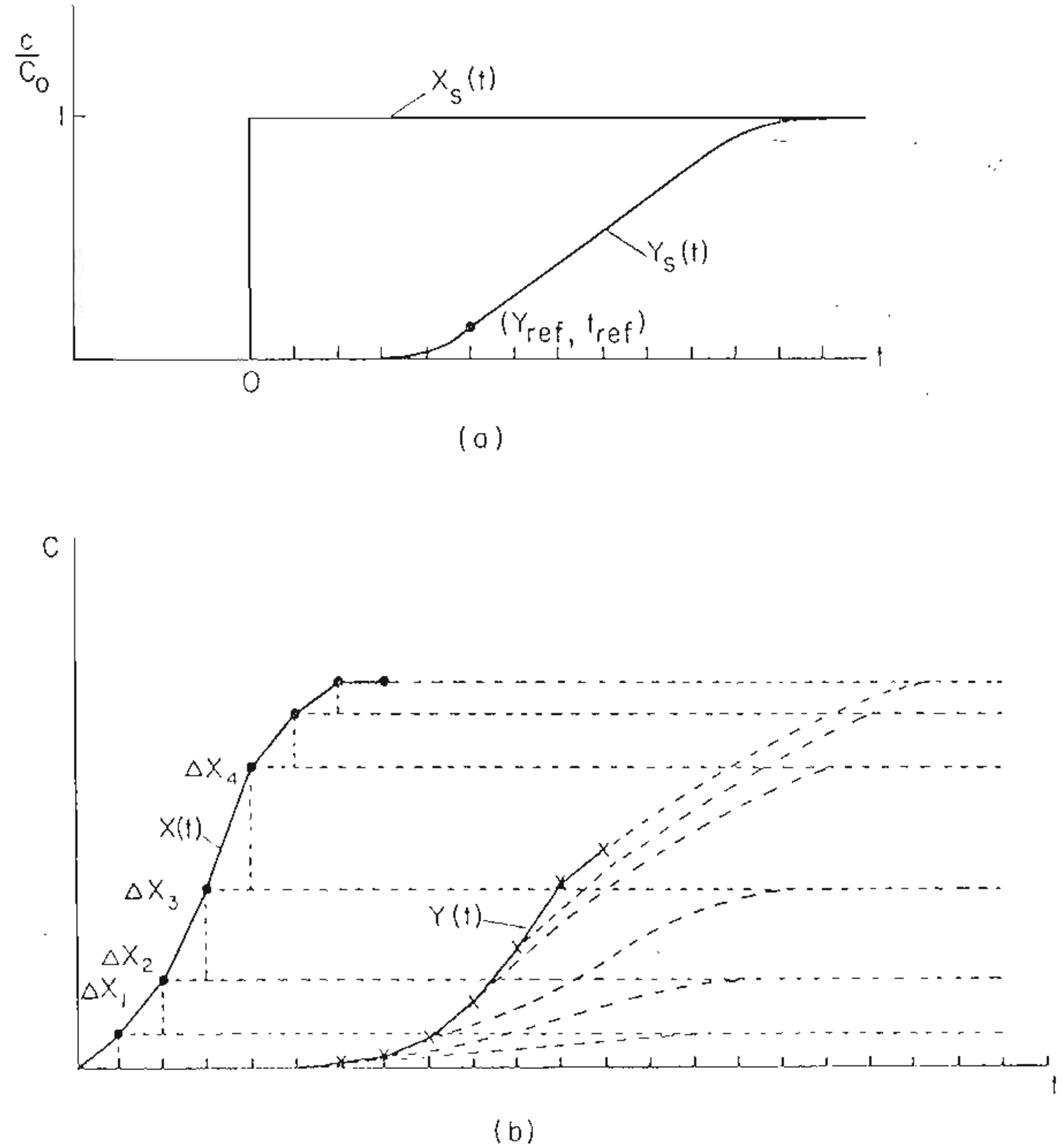

FIGURE 8. (a) SYSTEM STEP RESPONSE, AND (b) RECORDED OUTPUT WITH EQUIVALENT INCREMENTAL STEP INPUT

$$y(t) = \int_0^t y_s(t-\tau)\,\frac{dx}{d\tau}\,d\tau. \tag{7}$$

If the integrand is sufficiently simple, the equation can be analytically inverted to obtain $dx/d\tau$ as a function of τ and, hence, $\dot{x}(t)$. In practice, this is usually difficult, and one resorts to numerical techniques (Bellman et al., 1966)

In the present case, $y(t)$ is known (measured), and $x(t)$ is to be determined. The computational scheme proceeds as follows: On the measured response curve, $y_s(t)$ (Figure 8a), choose a reference point (y_{ref}, t_{ref}).* Move in time along the $y(t)$ record until the first measurable increase in y, y_1, is detected. This increase is interpreted as being generated by a step in x at a time t_{ref} earlier and of a magnitude, $\Delta x_1 = y_1/y_{ref}$. The step Δx_1 produces a corresponding response function which is subtracted from the entire remaining $y(t)$ record. One then advances to the next time step, observes the adjusted y_2, interprets it as a new Δx_2 at a time t_{ref} earlier and again subtracts the corresponding response function from the remaining $y(t)$ record. This procedure is repeated step by step in time to obtain $x(t)$, the input gas concentration as shown in Figure 8b.

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*Chosen such that y_{ref} is sufficiently small for resolution and sufficiently large for accuracy; a value of $y_{ref} = 0.1$ has been used successfully.

TRANSFER FUNCTION TECHNIQUE

With the same notation, we have, as before:

$$y_s(t) = \begin{cases} 0, \text{ for } t < t_L \\ 1 - [1 + (t-t_L)/t_c] \exp[-(t-t_L)/t_c], \text{ for } t \geq t_L , \end{cases} \quad (8)$$

and $$x_s(t) = 1, \text{ for } t \geq 0. \quad (9)$$

The Laplace transform of a function f(t) is (Hildebrand, 1962)

$$F(s) \equiv L \{f(t)\} \equiv \int_0^\infty \exp(-st)f(t)dt. \quad (10)$$

Hence,

$$Y_s(s) = \int_0^\infty [\exp(-st)]\{1-[1+(t-t_L)/t_c]\exp[-(t-t_L)/tc]\}dt,$$

$$= \frac{\exp(-st_L)}{s(1+t_c s)^2} , \quad (11)$$

and

$$X_s(s) = \int_0^\infty \exp(-st)(1)dt,$$

$$= \frac{1}{s} . \quad (12)$$

If we let G(s) denote the transfer function, then

$$G(s) \equiv \frac{Y_s(s)}{X_s(s)} ,$$

$$= \frac{\exp(-st_L)}{(1+t_c s)^2} , \tag{13}$$

which is invariant in the s-domain.

Since y(t) is usually known or treated numerically, it must be expressed numerically so as to allow Laplace transformation, division by the transfer function and inverse transformation. This can be done by fitting a second order polynomial $y_n(t)$, with continuous first derivative between successive data points. If y(t) is known at times $t_n = n\Delta t$ with discrete values y_n, it can be shown that

$$y_n(t) = y_n + a_n(t-t_n) + \frac{(y_{n+1} - y_n)}{\Delta t^2} - \frac{a_n}{\Delta t} (t-t_n)^2 , \tag{14}$$

where
$$a_n = \frac{2(y_n - y_{n-1})}{\Delta t} - a_{n-1} , \tag{15}$$

and
$$y(t) = \sum_{n=0}^{N} y_n(t). \tag{16}$$

where N is the total number of discrete data values. Accordingly, the Laplace transform of y(t) is

$$Y(s) = \frac{y_o}{s} + \frac{a_o}{s^2} - \frac{2a_o}{\Delta t s^3} + \frac{2(y_1 - y_o)}{\Delta t^2 s^3} + \sum_{n=1}^{N-1} \frac{2\exp(-sn\Delta t)}{\Delta t^2 s^3} A_n - R_N \exp(-sN\Delta t) \tag{17}$$

where $$A_n = (y_{n+1} - 4y_n + 3y_{n-1} + 2a_{n-1}\Delta t), \tag{18}$$

and $$R_N = \frac{y_N}{S} + \frac{a_N}{s^2} + \frac{a_N}{S^3\Delta t} . \tag{19}$$

For $t_L > \Delta t$, which is usually the case, $y_1=0$ and, since $y_o = a_o = 0$ by physical argument,

$$Y(s) = \sum_{n=1}^{N-1} \frac{2\exp(-sn\Delta t)}{\Delta t^2 s^3} A_n - R_N\exp(-sN\Delta t) . \tag{20}$$

To find the input gas concentration, the transformed input is determined using the transfer function, i.e.,

$$X(s) = Y(s)/G(s)$$

$$= \exp(st_L)(1+t_c s)^2 \sum_{n=1}^{N} \left\{\frac{2\exp(-sn\Delta t)}{\Delta t^2 s^3} A_n - R_N\exp(-sN\Delta t)\right\}. \tag{21}$$

The transformed input, X(s), is inverted to obtain the input in the time domain, i.e., with $t=m\Delta t$,

$$x(t) = L^{-1}\left\{X(s)\right\}$$

$$x(m\Delta t) = \sum_{n=N_o}^{N-1} A_n[(m-n+N_o)^2 + \frac{4t_c}{\Delta t}(m-n+N_o) + \frac{2t_c^2}{\Delta t^2}]u[(m-n+N_o)\Delta t], \tag{22}$$

for which

$$N_o = \frac{t_L'}{\Delta t}\text{ , where } t_L' = t_L + E\Delta t\text{, with } 0\leq E<1 \text{ such}$$

that N_o is an integer;

$$u[(m-n+N_o)\Delta t] = \begin{cases} 0 & \text{for } (m-n+N_o)<0 \\ 1/2 & \text{for } (m-n+N_o)=0 \\ 1 & \text{for } (m-n+N_o)>0 \end{cases} ;$$

and

$$0 \leq m \leq N-N_o-1.$$

This reduces finally to

$$x(o) = \frac{A_{N_o}\; t_c^2}{\Delta t^2}\text{ ,} \tag{23a}$$

and

$$x(m\Delta t) = \sum_{n=N_o}^{m+N_o-1} A_n\left[(m-n+N_o)^2 + \frac{4t_c}{\Delta t}(m-n+N_o) + \frac{2t_c^2}{\Delta t^2}\right] + \frac{A_{m+N_o}\; t_c^2}{\Delta t^2} \tag{23b}$$

$$\text{for } 1 \leq m \leq N-N_o-1.$$

This expression must be summed over n for each value of m. Thus, at each instant of time, the input to the gas sampling port is determined in terms of t_L, t_c, Δt and measured output data points.

List of Figure Captions

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