A COMPARISON OF VARIOUS MODELS FOR FITTING DATA TO THE RESULTS OF ENVIRONMENTAL MONITORING OF GASEOUS CONTAMINATION

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Two methods used for environmental contamination monitoring are: 1)Personnel monitoring (Houldsworth et al 1982) and 2)Static air sampling (Health & Safety Executive 1984). Gaseous Infra-Red Spectrophotometry is the most versatile method for the latter, but a major problem is that over large ranges of contaminant concentration the calibration curves are not linear. One solution is the use of a single point calibration method. If the point used is the maximum concentration measured then the calculated levels will always be higher than the actual levels. If the calculated level is less than the Threshold Limit Value (TLV) then the actual level will be less than the TLV. This leads to considerable over-estimation of actual levels.

This study has fitted calibration curves for nitrous oxide, ethylene oxide, perchloroethylene (Perklone), 1,1,2-trichloro-1,2,2-trifluoroethane (Arklone) and formaldehyde to various models using least squares regression analysis and applied them to the monitoring of nitrous oxide in dental clinics, formaldehyde and ethylene oxide from sterilisers, Arklone from ultrasonic surgical equipment cleaning plant and Perklone from dry cleaning equipment.

Experimental data were obtained using a MIRAN IR Gas Analyser Model 104 (Foxboro Analytical), which was calibrated using a closed loop system. Regression programmes were run on a BBC "B" microcomputer fitted with a Torch Z80 second processor. Daniel and Wood (1980) stated that when fitting equations to data, all relevant data must be used in estimating each constant, there must be reasonable economy in the number of constants and the methods used must estimate the error in Y.

Using linear regression analysis a plot of residuals against X shows a V-shape indicating a poor fit. Various linear transformations have been compared with non-linear models, using the method of Boxenbaum et al (1974) for 'goodness of fit' and economy of constants. Typical results for Perklone are presented in the table below.

Model	Correlation coeff.	Model	Correlation coefficient
$y=ax+b$	0.9684	$y=ax+bx^2+c$	0.9992
$y=ab^x$	0.8634	$y=ax+bx^2+cx^3+d$	0.9999
$y=ax^b$	0.9908	$y=ax+bx^2+cx^3+dx^4+e$	0.9999

Using the method of Boxenbaum et al (1974) it was shown that the cubic model gave the most significant fit, using the minimum of constants. Similar results were obtained for the other gases studied.

The above models have been compared with the one point calibration method for systems in which the levels of contaminant vary greatly. Using the regression analysis model for levels of Nitrous Oxide ranging from 1ppm to 9000ppm, a more accurate estimate of the concentration was obtained over the full range and an indication of the errors was obtained. Below 100ppm the one point calibration method resulted in errors of up to 50% in the calculated concentrations.

The method presented is simple, more accurate than the one point calibration method and gives an estimate of the error in the measurement.

Boxenbaum, H. G. et al (1974) J.Pharmacokin.Biopharm. 2: 123-148

Daniel, C. & Wood, F. S. (1980) Fitting equations to data. Computer analysis of multifactor data. John Wiley & Sons.

Health & Safety Executive (1984) Monitoring strategies for toxic substances. Guidance Note EH42

Houldsworth, H. B. et al (1982) Anaesthesia 37: 467-468