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Project Summary

Sampling Air for Gaseous Organic Chemicals Using Solid Adsorbents. Application to Tenax

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A simple input-output model for a two-phase flow system with fixed bed was applied to Tenax adsorption of atmospheric contaminants. The model fit laboratory data acceptably and relationships with previous approaches were stated. Chromatographic retention volumes are used in this model which provides a means of scaling adsorbent bed dimensions and flow rates to preserve desired output characteristics.

Suggestions are made about how to use the model for rational sampling design when quantitative information is needed. Practical limitations of field operations and fundamental knowledge and the need to evaluate every datum lead to practical suggestions for sampling. At least two samples collected simultaneously but at very different flow rates are suggested as necessary for quantitative work.

This Project Summary was developed by EPA's Environmental Monitoring Systems Laboratory Research Triangle Park, NC, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

Solid adsorbents are very convenient to use in field sampling and therefore have been employed extensively to concentrate trace organic pollutants in sampling ambient air. It was usual to assume that standard chromatographic theory could be applied. Since the main objectives of chromatography are not the same as those of field sampling with solid adsorbents, that theory was not developed with the goal of solving the practical problems of establishing field sampling procedures. Variables that are critical in the field situation are not explicitly handled in a convenient way and a huge fundamental data base is needed for application.

The objectives of this work were:

1. To obtain a simple alternative model which incorporates a minimum number of adjustable parameters and establishes a relationship among important sampling variables:
   - (a) weight of adsorbent
   - (b) adsorbent bed (sampling tube) geometry
   - (c) flow rate
   - (d) input concentration to the adsorbent bed
   - (e) adsorbent bed output concentration
   - (f) elapsed sampling time
2. To test the accuracy of the function obtained in describing a few simplified controlled laboratory experiments; and
3. To design a simple practical scheme for sampling and data interpretation which also can provide evidence of consistency in the results.

Procedure

The model investigated can be written as:

$$\ln \frac{C}{C_o} = \frac{K_o L}{V_L}\left[\frac{t}{t_s} - 1\right]$$

C is the bed's exit concentration at elapsed time t, g/cm^3

C_o is the bed inlet concentration, g/cm^3

K_o is a pseudo first-order rate constant, min^{-1}

L is the adsorbent bed length, cm

V_L is a superficial flow velocity, cm/min

t is the elapsed time after beginning of sampling, min.

t_s is the elapsed time required to reach the adsorbing capacity of the bed. Under restricted conditions it is equal to ratio of the familiar chromatographic retention volume to the volumetric flow rate.

The model is an approximate relation applicable to any adsorbent. However, its validity is limited to a range of elapsed times from perhaps $0.1 < \frac{t}{t_s} < 0.8$.

The utility of the model was tested by simulated sampling using a permeation tube system to supply known concentration of cleaned pollutant doped air at various flow rates. Flame ionization detection of the output of the Tenax cartridge was utilized to obtain a relationship between elapsed time and concentration of the pollutant in the effluent from the cartridge. The effects of changes in concentration temperature, flow rate, and bed size were investigated. Chloroform, trichloroethylene, benzene, tetrachloroethylene, toluene, 1,2-dichloroethane and 1,3-dichloropropane were used in the experiments.

Computation of the retention volume and K_o from the constants of the empirical fits was done by simple rearrangement of the basic equation to match the empirical form and identifying the appropriate collection of variables with the empirical constants.

Results

Agreement of computed retention volumes with published values was generally within ±25 percent. No concentration dependences or changes due to the presence of another substance were observed at 38°C. Both effects were observed on the same chemical systems at 10°C. K_o was less well behaved and characterized but exhibited a typical value of about 200 min^{-1}.

Conclusions

The model is capable of giving a reasonable and compact description of the sampling behavior of the Tenax cartridges over a range of variables likely to be met in the field:

35 cm^3/min < flow rate < 500 cm^3/min

1.25 cm < bed radius < 0.6 cm

when

$$2 < \frac{\text{Bed Length}}{\text{Bed Radius}} < 4$$

and

$$30 \text{ cm/min} < \frac{\text{Flow Rate}}{\pi\,(\text{Bed Radius})^2} < 400 \text{ cm/min}$$

Recommendations

A suggested simplified approach for routine sampling is as follows:

1. Use a fixed cartridge size. (At present GC/MS sample desorbers limit severely the options with respect to cartridge size.)
2. Allow the single substance, whose determination is required and which has the smallest published retention volume at 38°C (100°F), control the sampling calculations. If necessary, divide the list into ranges of retention volumes and sample independently for each range.
3. The desired sample averaging time is usually specified by the situation.
4. Compute a flow rate conservatively using the model and an acceptable value of C/C_o. Or, more simply, use the published retention volume divided by the desired sampling time. If ambient temperatures are expected to be cool, use the value computed. If they are near 29°C (85°F) or higher, use one-half the computed value.
5. Present evidence in every situation of the data credibility. Complete every sampling in at least duplicate (parallel) at different flow rates, e.g., the flow rate computed in 4 above and another at perhaps half of that value. "Agreement" of the analyses on duplicate samples would be an indication of adequate retention.

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The complete report, entitled "Sampling Air for Gaseous Organic Chemicals Using Solid Adsorbents. Application to Tenax," (Order No. PB 82-262 189; Cost: $8.50, subject to change) will be available only from:

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