Extended Range VOC Measurements in Ambient Air using Multi-Sorbent Diffusive Monitoring Tubes

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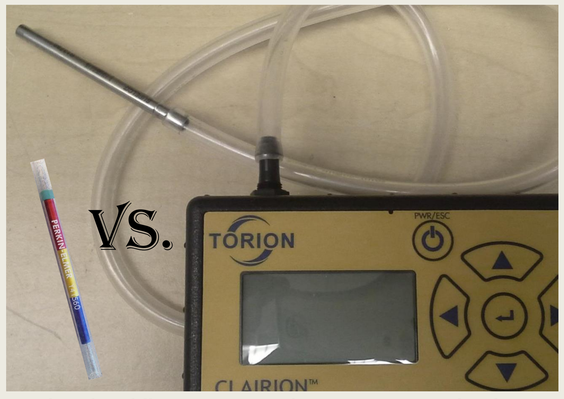
1 Introduction

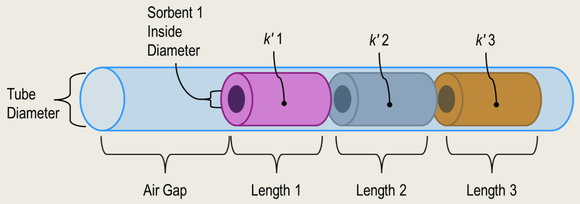
Ambient air monitoring is becoming more challenging as the need for more information on more compounds at lower detection limits increases. Part of the challenge is keeping analytical methods simple and cost effective. Sorbent tube sample collection followed by thermal desorption-gas chromatography is becoming increasing popular. Diffusive sampling is especially attractive as it is both very simple and low cost. However, traditional diffusive monitoring is limited to a single sorbent, which limits the volatility range of analytes. The multi-sorbent diffusive monitoring tubes described in this paper provide a very easy and cost effective means of collecting and analyzing wide volatility range ambient air samples.

Advantages of Multi-Sorbent Diffusive Monitoring Tubes

- Up to weeks of sampling time possible
- Allows a wider range of compounds to be analyzed
- Designed to be used without a pump
- Selective sorbent protection, allowing the use of unique sorbents that are intolerant of certain chemicals
- Customizable, giving the expert user a great amount of flexibility in tube design



Multi-sorbent diffusive monitoring tube vs. Torion pump with multi-sorbent packed bed thermal desorption tube.

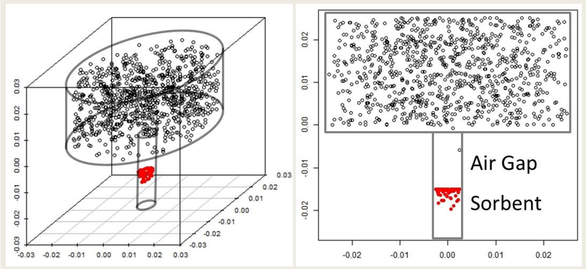


Theoretical construction of a MSDM tube, with parameters and dimensions modeled in simulation

2 MCMC Simulation

A Markov chain Monte Carlo (MCMC) simulation was constructed to determine the position of the molecules versus the parameters. The parameters examined were:

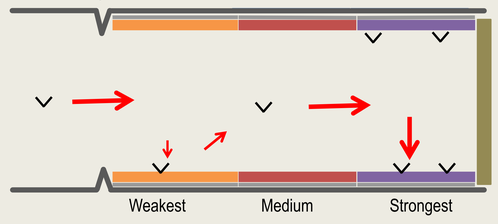
- Time
- Molecular constants
- Air gap length
- k' capacity factor of each sorbent
- Dimensions of each sorbent coating



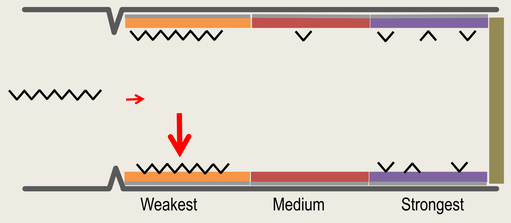
Position of molecules in simulation after 0.1 seconds. Red molecules are bound to the adsorbent.

3 Simulation Results

Light Molecules diffuse faster into the tube, and are more likely to desorb from weak sorbents.



Heavier molecules diffuse slower into the tube, and are less likely to desorb from weak sorbents.



Weaker sorbents 'protect' stronger sorbents from:

- Larger molecules
- Polar Molecules
- Others by design

4 Model

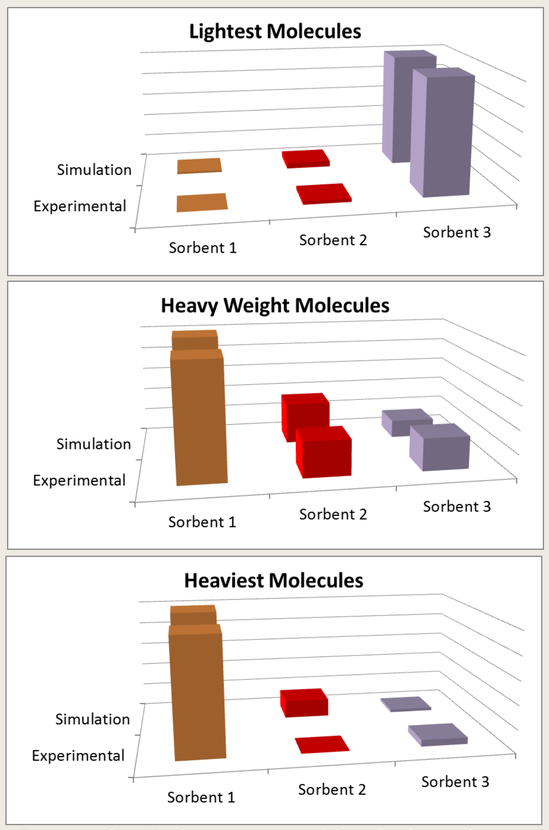
It was found that the best model was one that estimated the proportion of molecules that made it past a sorbent (or air gap) to the next sorbent. This proportion was then transformed with the logit transformation, and applied to a linear model

$$\log(\mathbf{p}/\mathbf{1}\text{-}\mathbf{p}) = \mathbf{X\beta} + \boldsymbol{\varepsilon}$$

where **p** is a vector of proportions of molecules that diffused to the next sorbent, **X** is a matrix of parameters, **β** is the vector of coefficients, and **ε** is the error.

5 Experimental

Prototype sorbent coated tubes were provided by Millipore Sigma. The tubes were extensively tested for functionality and verification of the simulation model.



Experimental vs. Simulation: proportion of the molecule in each sorbent versus molecular weight

6 Future Work

Development of this technology will yield a small, cost effective, customizable, wide-range solution to air monitoring.

The laboratory results were predicted very well with the model, indicating a good model and sound theory. With a verified model, the parameter space can be further explored.

Future work will include testing a wider range of sorbents and sorbent geometries, and a wider range of conditions. This will allow a more in-depth characterization of the simulation model.

This project is in the research phase, and commercially available multi-sorbent diffusive monitoring tubes are not yet available. Beta testing phases will include outside organizations to verify and validate functionality, as well as give input into the design.

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7 Summary

The multi-sorbent diffusive monitoring tube technology will increase the functionality and performance of thermal desorption tubes:

- No pump needed
- Can be used with a wide range of analytes
- Can be customized for specific applications
- Long sampling times possible
- Many sorbent choices
- Designed sorbent layering makes previously impractical sorbents possible
- Small
- Convenient
- Discrete
- Compatible with current thermal desorption instruments
- Post-adsorption disassembly possible for a customized GC chromatogram

More research and testing must be done before a product can be produced.

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