Thermally Controlled Gas Sorption

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Introduction

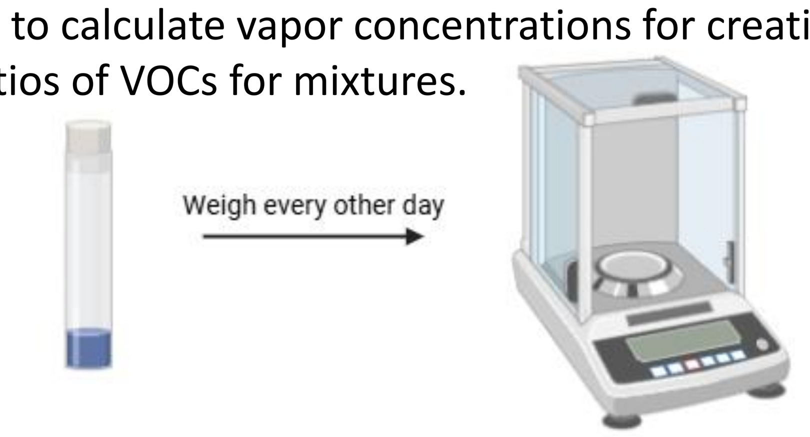
Better portable and low-cost methods are needed for gas sensing and separation with key applications in environmental monitoring and industrial processes.

Volatile organic compounds (VOCs) are carbon-based chemicals and common pollutants. This study examines how thermal parameters, including ramp rate and oven temperature, influence adsorption and desorption dynamics.

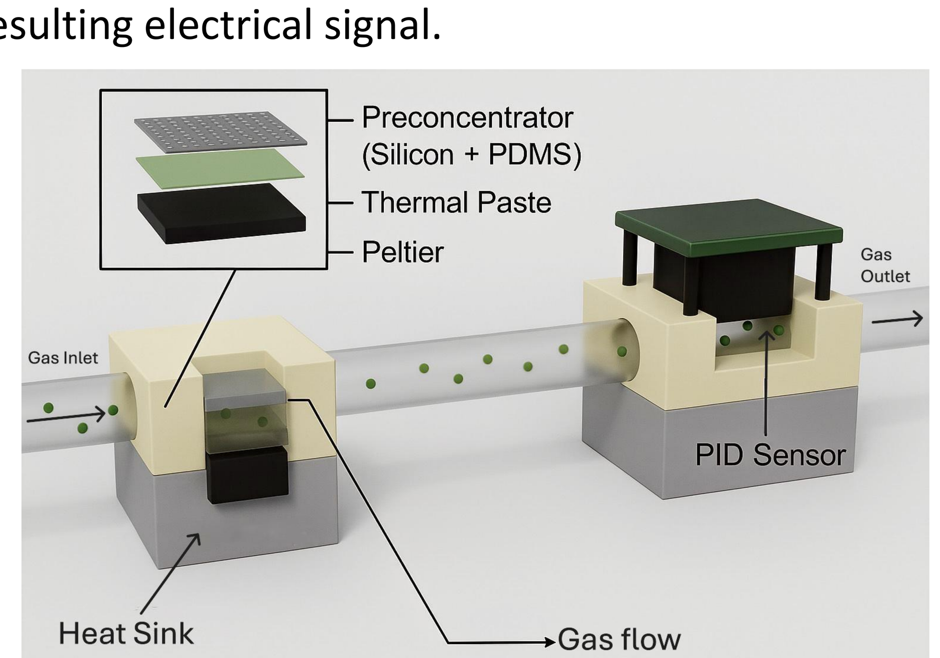
This study evaluates the impact of VOC (benzene, toluene, ethylbenzene, and o-xylene) concentration on separation performance, to determine the most effective parameters for resolving VOC mixtures.

Experimental Set-Up

Permeation tubes with different VOCs were placed in the Vertical Owlstone Vapor Generator (V-OVG) and weighed every other day to determine diffusion rates. These rates were used to calculate vapor concentrations for creating desired ratios of VOCs for mixtures.



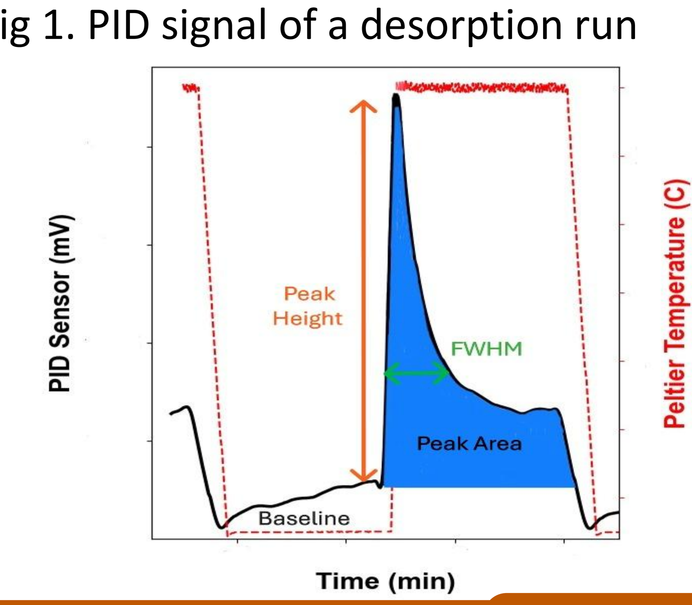
In this setup a controlled vapor stream was generated using a V-OVG oven filled with permeation tubes. The system released VOC vapors into a carrier gas stream flowing toward a Photoionization Detector (PID). The PID detects the compound by ionizing molecules with UV light and measuring the resulting electrical signal.



After calibrating permeation tubes to new concentrations, desorption runs were performed for individual VOCs and mixtures at various parameters. The resulting PID signal over time provided thermal profiles for each condition.

Methods

Fig 1. PID signal of a desorption run



Relative Peak Height: Highest concentration of VOC released at a time

Peak Area: Represents total amount of VOC desorbed

FWHM (Full Width at Half Maximum): Indicates how broad the peak is and how quickly VOC was released

Baselines: Stable PID signal when no VOCs are being released

Max Peak time: Allows for comparing how quickly different VOCs or mixtures desorb

Ramp Rate: Rate of temperature increase

Experimental Results

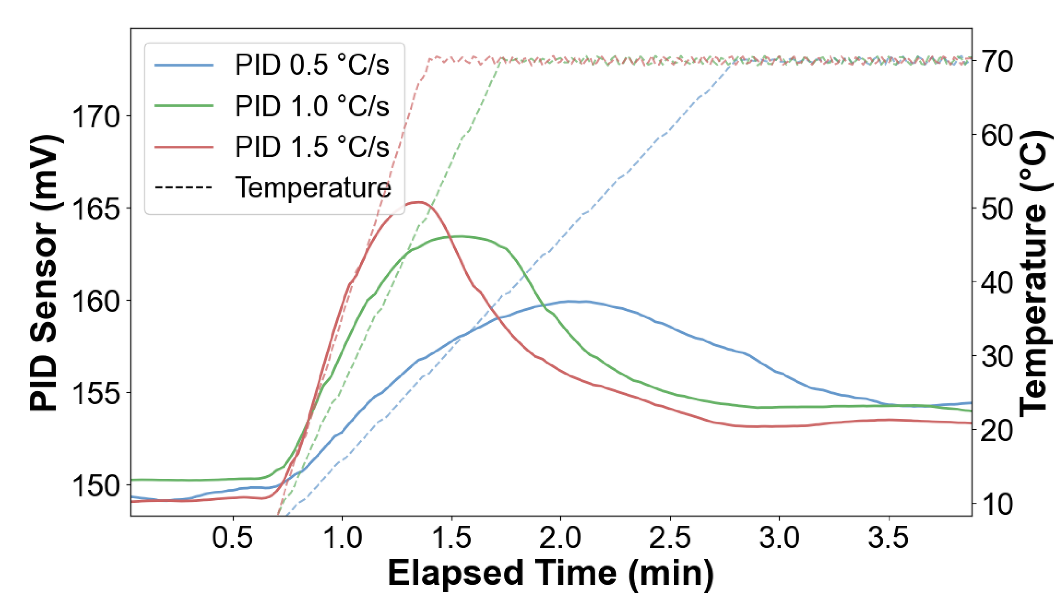


Fig 2. Full peak comparison of toluene 1.57 ppm PID signal at different ramp rates. As ramp rate increased, so did relative peak height. Peaks were also sharper at higher ramp rates; however, lower ramp rates allow for better separation

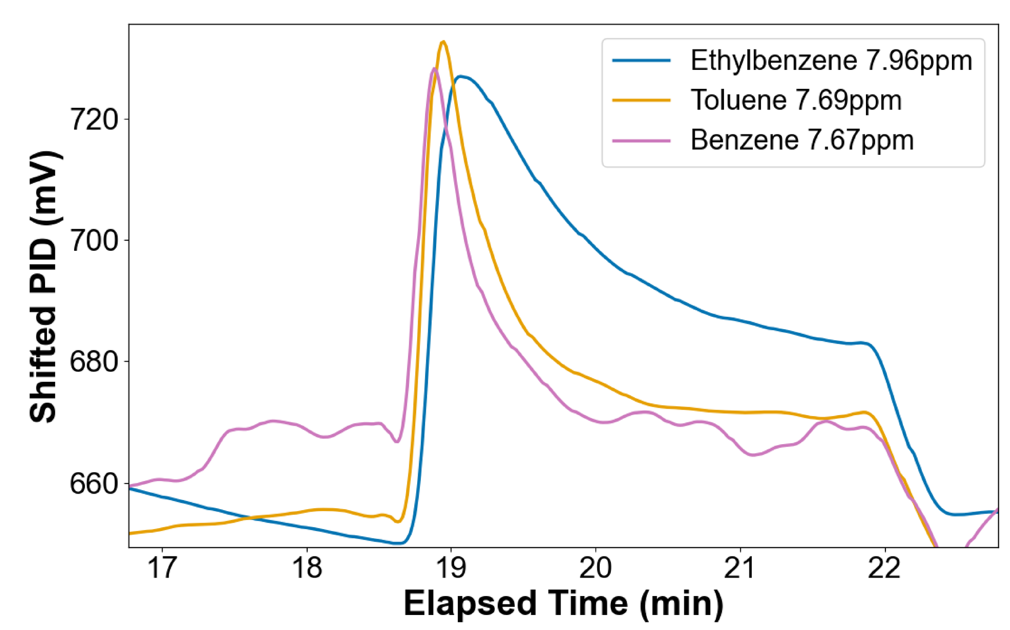


Fig 3. Comparison of different volatile organic compounds at approximately the same concentration. More volatile compounds desorb faster, with peaks reaching their maximum more rapidly. Benzene shows more noise in the system then toluene and ethylbenzene.

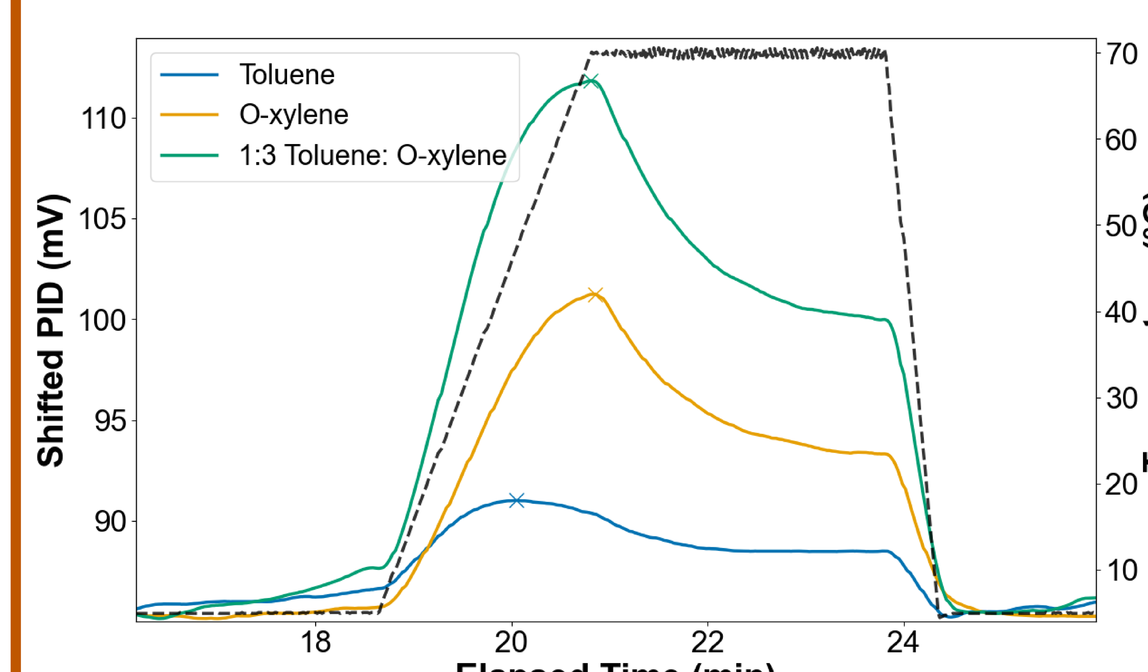


Fig 4. Peak comparison of individual compounds and a 1:3 toluene: o-xylene mixture at 0.5°C/s. toluene 0.55 ppm and o-xylene 1.69 ppm. The stronger o-xylene signal dominates, causing the mixture's decay and peak to closely resemble o-xylene 's.

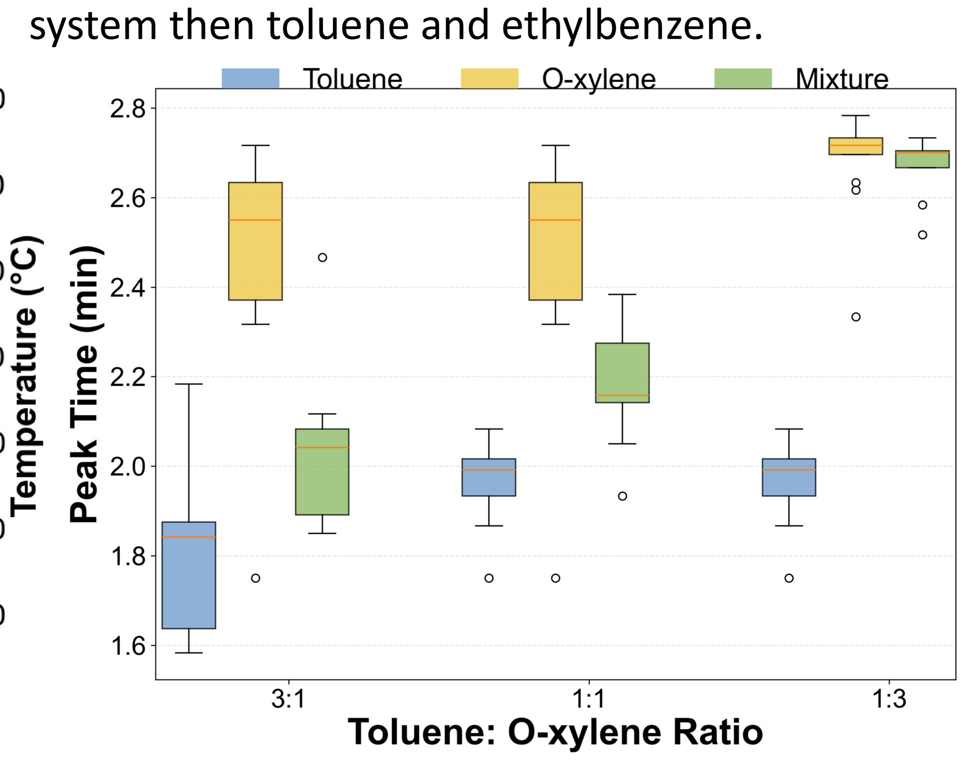


Fig 5. Relative peak times for individual compounds and toluene: o-xylene mixtures at various ratios. Peak separation was greatest at 3:1 and 1:3 ratios, with the 1:3 mixture showing less variability across all compounds.

Future Work

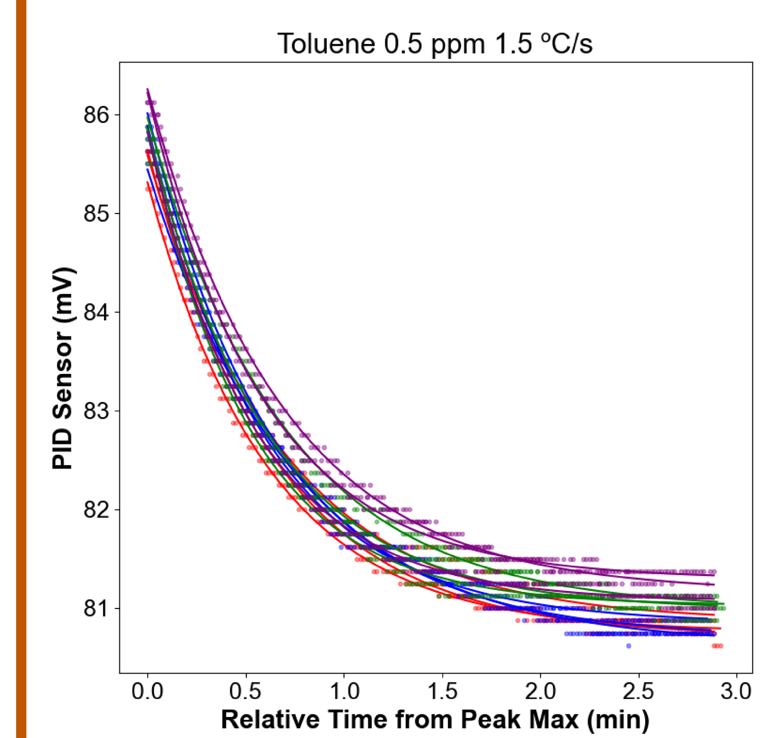


Fig 6. Desorption behavior of toluene 0.5 ppm. Data points are shown with a fitted model

$$y = Ae^{-k_0 t\left(e^{\frac{E_d}{RT}}\right)} + C$$

to better understand how VOCs releases over time.

Future work could explore how the rate constant or activation energy changes with different compounds or temperatures.

At ramp rates below 1°C/s, benzene produces noisy signals and o-xylene gives minimal response. Further examination of concentration is needed to determine the detection limits for effective gas separation.

Acknowledgments

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References

Selective Detection of Volatile Organics in a Mixture Using a Photoionization Detector and Thermal Desorption from a Nanoporous Preconcentrator
Joshua Prestage, Coco Day, Shamus L.G. Husheer, William T. Winter, Wah O. Ho, John R. Saffell, and Tanya Hutter
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