The relationship between liquid- and vapor-phase concentrations for ketone odorants diluted in mineral oil using a photoionization detector-based approach.

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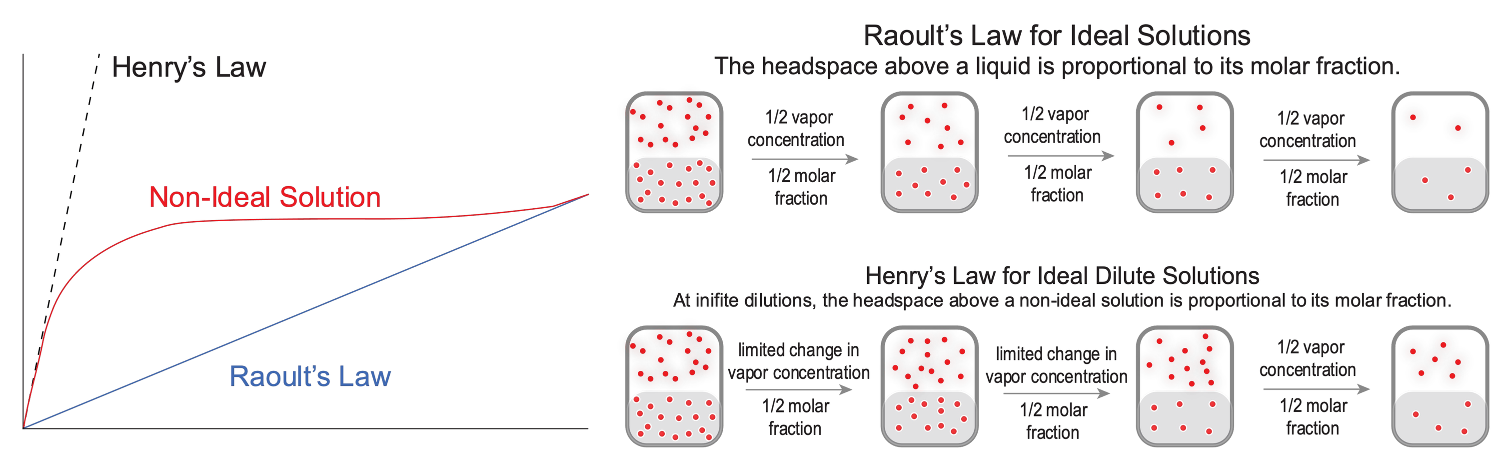
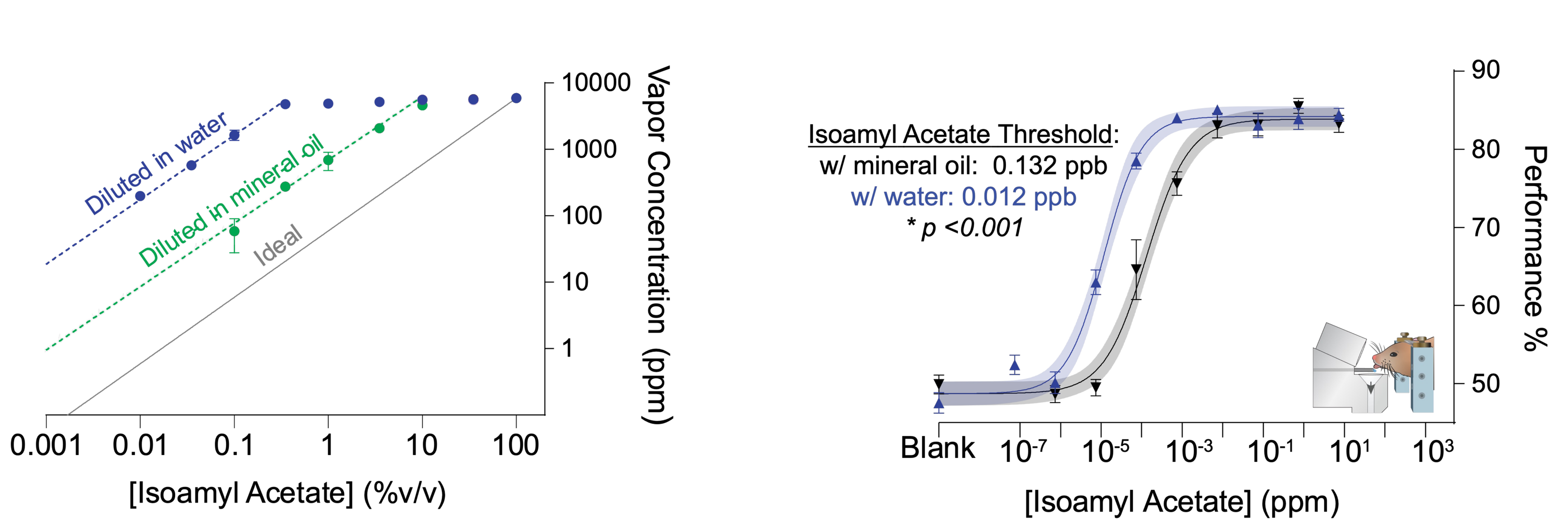
Introduction

- Odor studies rely on liquid dilutions to manipulate the vapor-phase concentrations of volatile odorants
- **Goal**: Analyze the relationship between liquid- / vapor-phase concentrations of ketones using a photoionization detector (PID)
- PIDs use high-intensity ultraviolet light to ionize the volatiles resulting from a liquid dilution, yielding a current that is proportional to the vapor-phase concentration
- We are creating a large archive of a vast amount of odorant concentrations in which ketones will be included
- The liquid-vapor-phase equilibrium equations can be used by other researchers to obtain accurate vapor-phase ketone concentrations.

Odorants Rarely Follow the Law of Proportionality

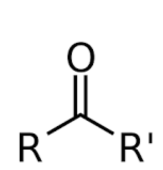


Vapor Phase Concentration is Dependent upon the Solvent



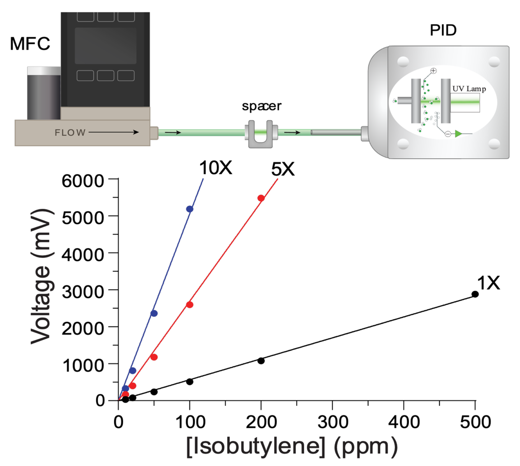
Ketone Odorants

- Ketones are volatile chemicals that are typically described as having fruity or solvent-like odors and are frequently used in olfactory research
- Characterized by a carbonyl functional group with two hydrocarbon substituents

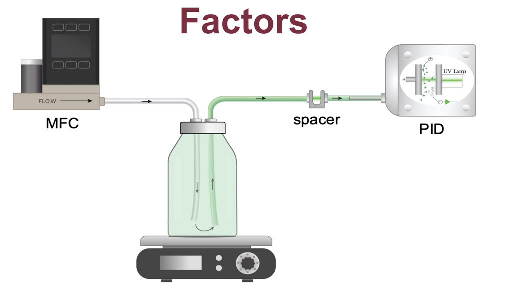


Methods

Photoionization Detector Calibration

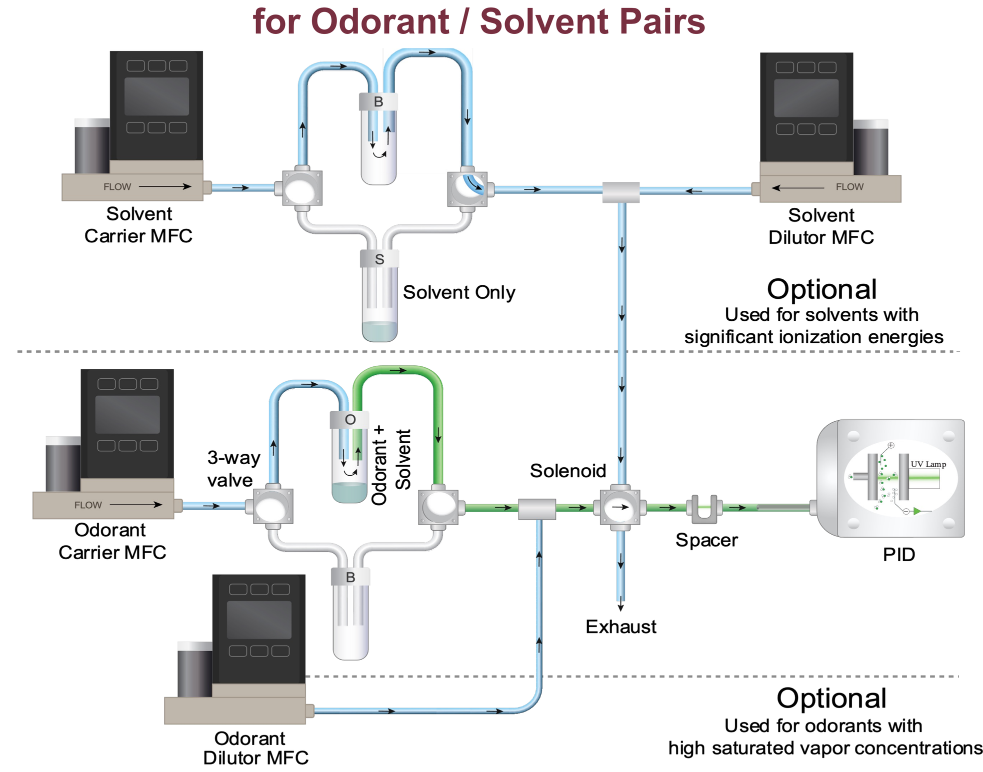


Measuring PID Correction Factors

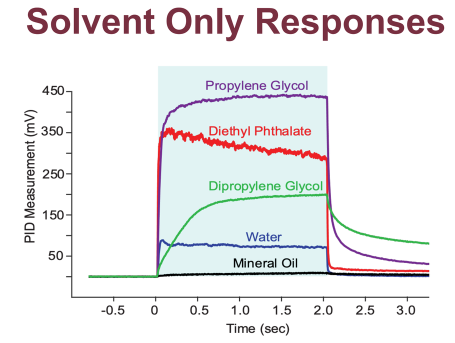


Odorant	Vapor (PPM)	Calibrated PID Resp. (PPM)	Measured CF	Other PID CFs
Propyl Acetate	1871	589	**3.18**	3.0 ~ 3.5
Butyl Acetate	1608	644	**2.49**	2.4 ~ 2.6
Isobutyl Acetate	1590	570	**2.79**	2.0 ~ 2.6
Pentyl Acetate	1435	659	**2.18**	~2.3
Isoamyl Acetate	1419	722	**1.97**	1.5 ~ 2.1
Hexyl Acetate	1278	659	**1.94**	NA

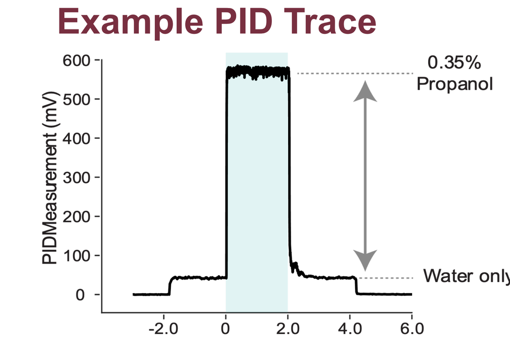
Measuring the Liquid -/ Vapor-Phase Relationships for Odorant / Solvent Pairs



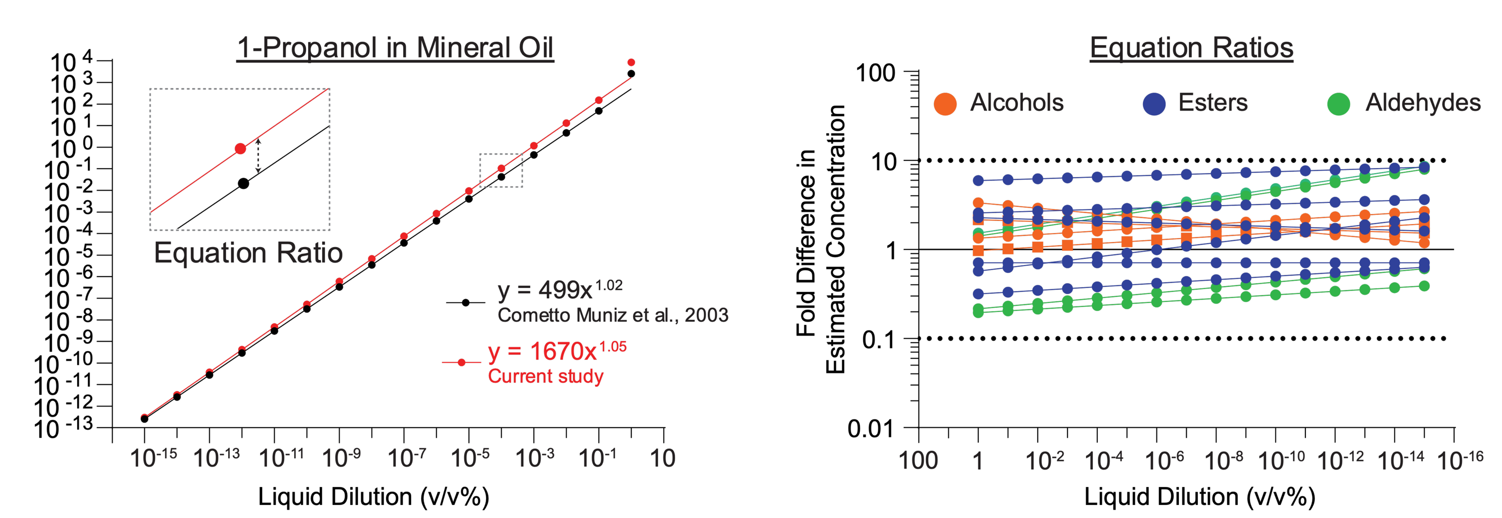
Solvent Only Responses



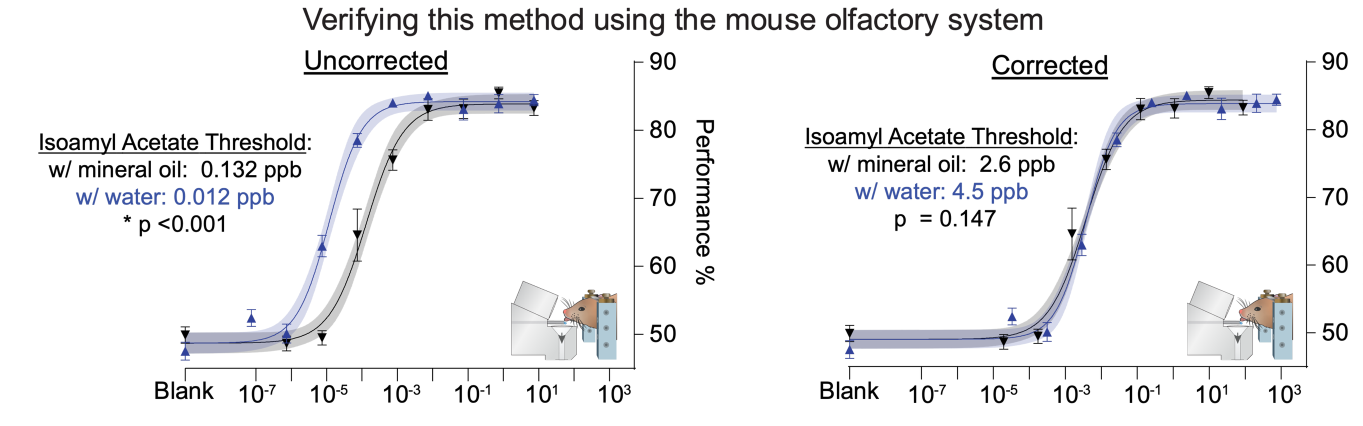
Example PID Trace



Validating the Method

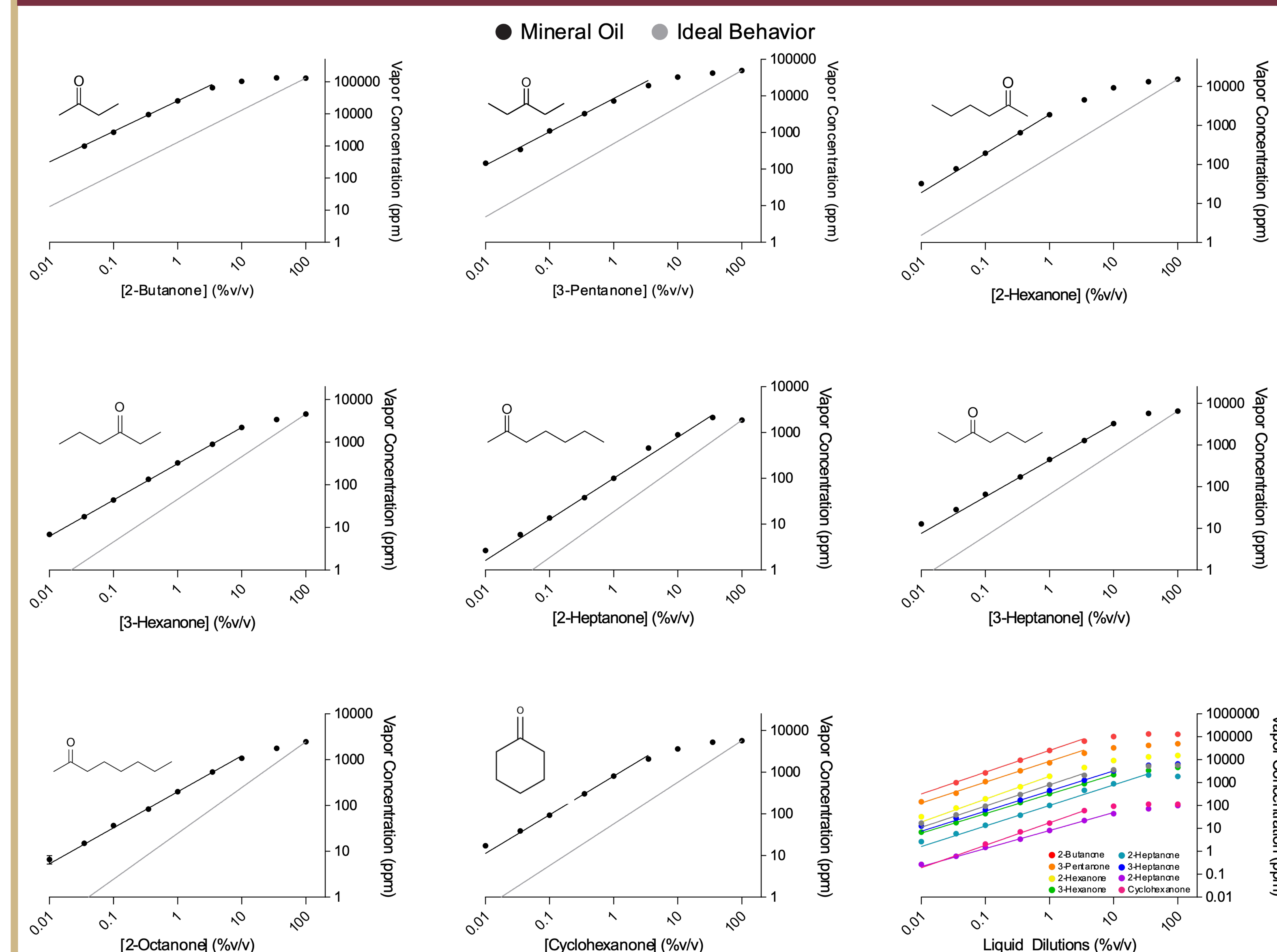


Verifying this method using the mouse olfactory system



Our liquid-/vapor-phase equilibrium equations successfully corrected for behavioral sensitivity differences observed in animals tested with the same odorant in different solvents.

Results



Odorant	Ideal Behavior	Mineral Oil
2-Butanone	$y=1296x^{1.00}$	$y=25377x^{0.95}$
3-Pentanone	$y=496.1x^{1.00}$	$y=8508x^{0.91}$
2-Hexanone	$y=152.6x^{1.00}$	$y=1889x^{1.00}$
3-Hexanone	$y=45.75x^{1.00}$	$y=312.3x^{0.85}$
2-Heptanone	$y=18.7x^{1.00}$	$y=100.3x^{0.90}$
3-Heptanone	$y=65.1x^{1.00}$	$y=429.4x^{.88}$
2-Octanone	$y=24.6x^{1.00}$	$y=199x^{0.79}$
Cyclohexanone	$y=57.0x^{1.00}$	$y=798.9x^{0.93}$

Summary & Future Applications

- Diluted ketones exhibit near ideal behavior in mineral oil.
- PID is reasonably accurate at measuring liquid- / vapor-phase equilibrium relationships in different solvents.
- Future experiments will analyze additional ketones in different solvents.
- This data will be included in a practical archive of liquid/vapor-phase equilibrium equations of different odorants in various solvents.

References

- Cometto-Muñiz, J.E., Cain, W.S., and Abraham, M.H. 2003. Quantification of chemical vapors in chemosensory research. Chem Senses. 28:467–477.
- Jennings, L., Williams, E., Caton, S., Avlas, M., & Dewan, A. (2022). Estimating the relationship between liquid- and vapor-phase odorant concentrations using a photoionization detector (pid)-based approach. *Chemical Senses*, *48*. https://doi.org/10.1093/chemse/bjac038