AQUALAB
by Addium

EDUCATION GUIDE

Volatile Ingredients and a_w

A GUIDE TO CHOOSING THE BEST WATER ACTIVITY SENSOR FOR YOUR NEEDS.

AQUALAB produces instruments with three types of water activity sensors: a dew point sensor, a capacitance sensor, and a tunable diode laser (TDL) sensor. Each sensor has a unique way of measuring water activity (a_w) and each sensor varies in its ability to accurately measure in the presence of interfering volatile compounds (VCs).

Traditionally the dew point sensor is the fastest and most accurate sensor, but it can struggle in the presence of VCs due to their co-condensation onto the chilled mirror. The capacitance sensor is able to overcome the condensation issue, but this type of sensor generally has a lower precision, a higher data acquisition time and can be poisoned by certain compounds (some alcohols have been shown to interfere). The TDL sensor was specifically designed to measure water activity in the presence of other volatile compounds and is the flagship instrument for this purpose.

This guide will cover many common ingredients found in food products or other consumables that you may encounter while developing recipes or formulations. The goal of this guide is to aid the end user in choosing an instrument that will best fit their needs for determining water activity across a wide spectrum of use cases. While many of the samples presented in this report contain volatile compounds or are themselves volatile, instrument performance varies greatly depending on the processing of these compounds or ingredients. Best and worst case scenarios will be presented when applicable and an instrument recommendation will be made based on typical use cases.

Procedure

Prior to running any samples, all instruments were calibrated and verified against a set of known a_w standards. A representative sample of each ingredient was analyzed in a minimum of three individual instruments per sensor. Each sample was run until the instrument gave three readings within the sensor specification (Δa_w accuracy: dew point ±0.003, capacitance ±0.015, and TDL ±0.005).

The spices used in this study were taken from a quickly rotating bulk foods section at a grocery store. The essential oils were sourced from a USDA organic supplier and marked for internal use. The other food additives used were all ACS reagent grade. All spices and essential oils were measured undiluted directly from their packaging. The other food additives were diluted with water to test a range of mass concentrations. No substrates were used - generally speaking additional substrates may lessen sample volatility.

Results

The data collected was reviewed to determine whether or not volatile compounds were interfering with the water activity measurements. Given the TDL sensor's performance in the presence of volatile compounds, it was taken as the most accurate and set as the standard for comparing the other instruments. Using our sensor specifications, the additive Δa_w was taken as the acceptable error. The stated sensor specification for the TDL is $\Delta a_w \pm 0.005$ and therefore the maximum acceptable error between two TDL sensors is the sum of the errors, or $\Delta a_w \pm 0.01$. Generally speaking a $\Delta a_w < 0.01$ corresponds to a difference between instruments of 1-2% and is within the normal instrumental error. An error between $\Delta a_w \pm 0.01$ and 0.02 (3 and 5%) suggests some

interference may be present, and above 0.02 (5%) the readings are significantly different and above twice the acceptable error, likely due to interfering volatile compounds. Three levels of recommendations are given in the table below. If an ingredient gives good performance at all concentrations then a dew point sensor is the best choice (non-interfering). If the sample is sufficiently volatile that it can cause issues with the dew point sensor at high concentrations, but fairs well at lower concentrations then a dual block instrument is recommended (concentration dependent). If the ingredient causes inaccurate readings even at low concentrations then a TDL sensor is recommended (highly interfering).

These data points represent samples that a consumer would encounter. Fresh spices and herbs, perhaps directly from a producer, may have higher concentrations of interfering volatile compounds and will not perform to the same level of accuracy as our samples. Furthermore, volatile compound content of herbs and spices can vary widely depending on plant species, handling and processing, and storage and age. A literature review of the potential volatile compounds is found in the volatility profile of spices.

AQUALAB Devices & Sensors

AQUALAB 3	Dew Point and Capacitance Sensors
AQUALAB 4TE	Dew Point
AQUALAB TDL2	Tunable Diode Laser (TDL)

INGREDIENT NAME	EXPERIMENTAL RESULTS† AND VOLATILITY PROFILE	INSTRUMENT RECOMMENDATION DEW POINT, TDL, CAPACITANCE
DRIED SPICES & HERBS		
ALLSPICE, GROUND	Dew point sensor reads on average 0.014 (3%) higher than TDL. This is outside the range of acceptable accuracy. Up to 6% mass is essential oil. The major component is eugenol.[1]	**Capacitance or TDL** In low concentrations a dew point sensor should be sufficiently accurate. If higher levels of allspice are used occasionally then a capacitance sensor may help. If fresh allspice is a major component then a TDL should be considered.
BASIL	Dew point sensor reads on average 0.025 a_w (6%) higher than TDL. This is far outside the range of acceptable accuracy. Up to 2% mass is essential oil. The major component is linalool.[2] Lots of variation among species.	**Capacitance or TDL** TDL is best for samples with substantial amounts of basil.

BLACK PEPPER, GROUND	Dew point sensor gives contaminated mirror error. 0.4%-7% of mass is essential oil. The major component is piperine.[3]	**TDL** TDL is best for samples with substantial amounts of fresh ground black pepper.
CAYENNE, GROUND	Dew point sensor reads 0.007 a_w (2%) higher than TDL. Difference is below the combined error threshold.	**Dew Point** Dew point sensor gives good accuracy.
CINNAMON, GROUND	Dew point sensor reads 0.01 a_w (2%) higher than TDL. Difference is at the combined error threshold. Cinnamaldehyde is a major component of essential oil[4]	**Capacitance or TDL** In low concentrations a dew point sensor should be sufficiently accurate. If higher levels of cinnamon are used occasionally then a capacitance sensor may help.
CLOVES, WHOLE	Dew point sensor reads 0.03 a_w (8%) higher than TDL. This is far outside the range of acceptable accuracy. 45-90% of the essential oil is eugenol.[5]	**TDL** TDL is best for samples with substantial amounts of clove.
CORIANDER SEEDS, GROUND	Dew point sensor reads 0.02 a_w (5%) higher than TDL. This is far outside the range of acceptable accuracy. 0.5-2.5% of mass is essential oil. The major component is linalool.[6]	**TDL** TDL is best for samples with substantial amounts of ground coriander.
CUMIN, GROUND	Dew point sensor reads 0.01 a_w (2%) higher than TDL. Difference is at the combined error threshold. Up to 3% of mass is essential oil. The major component is cuminaldehyde.[7]	**Capacitance or TDL** In low concentrations a dew point sensor should be sufficiently accurate. If higher levels of cumin are used occasionally then a capacitance or TDL sensor may help.
GARLIC, POWDER	Dew point sensor reads 0.01 a_w (3%) higher than TDL. Difference is at the combined error threshold.	**Capacitance or TDL** In low concentrations a dew point sensor should be sufficiently accurate. If higher levels of garlic powder are used occasionally then a capacitance or TDL sensor may help.

GINGER, POWDER	Dew point sensor reads 0.01 a_w (3%) higher than TDL. Difference is at the combined error threshold. Up to 3% of the weight of fresh ginger is essential oil. These are primarily zingerone, shogaols, andgingerols.[8] Lots of species variation, and the drying technique plays a large role in what compounds are present.	**Capacitance or TDL** In low concentrations a dew point sensor should be sufficiently accurate. If higher levels of ginger powder are used occasionally then a capacitance or TDL sensor may help.
MEDIUM CHILI, POWDER	Dew point sensor reads 0.005 a_w (1%) higher than TDL. This is below the combined error threshold.	**Dew Point** Dew point sensor gives good accuracy.
NUTMEG, GROUND	Dew point sensor reads 0.014 a_w (3%) higher than TDL. Difference is above the combined error threshold. Up to 1.4% of mass is essential oil, mainly myristicin.[9]	**Capacitance or TDL** In low concentrations a dew point sensor should be sufficiently accurate. If higher levels of nutmeg are used occasionally then a capacitance sensor may help. TDL is best for samples with substantial amounts of ground nutmeg.
ONION, POWDER	Dew point sensor reads 0.003 a_w (1%) higher than TDL. This is below the combined error threshold.	**Dew Point** Dew point sensor gives good accuracy.
OREGANO	Dew point sensor reads 0.01 a_w (3%) higher than TDL. Difference is at the combined error threshold. Over 60 compounds, primarily carvacrol and thymol.[10] Lots of species variation.	**Capacitance or TDL** In low concentrations a dew point sensor should be sufficiently accurate. If higher levels of oregano are used occasionally then a capacitance or TDL sensor may help.
PAPRIKA, GROUND	Dew point sensor reads 0.008 a_w (2%) higher than TDL. Difference is below the combined error threshold.	**Dew Point** Dew point sensor gives good accuracy. If higher levels of paprika are used occasionally then a capacitance or TDL sensor may help.

SAGE	Dew point sensor reads 0.02 a_w (5%) higherthan TDL. This is far outside therange of acceptable accuracy. Numerous compounds including α-humulene, β-pinene, eucalyptol, and camphor.[11]	**TDL** TDL is best for samples with substantial amounts of sage.
SMOKED PAPRIKA, GROUND	Dew point sensor reads 0.008 a_w (2%) higher than TDL. Difference is below the combined error threshold.	**Dew Point** Dew point sensor gives good accuracy. If higher levels of paprika are used occasionally then a capacitance or TDL sensor may help.
WHITE PEPPER, GROUND	Dew point sensor reads 0.005 a_w (1%) higher than TDL. Difference is below the combined error threshold. White peppercorns differ from black peppercorns in that they are soaked in water and their skins removed, meaning many of the volatile compounds are lost.	**Dew Point** Dew point sensor gives good accuracy. If higher levels of white pepper are used occasionally then a capacitance or TDL sensor may help.
OTHER FOOD ADDITIVES		
ASCORBIC ACID	At all concentrations ascorbic acid can be accurately read by a dew point sensor. M.P. 190-192 °C, no appreciable vapor pressure at 25 °C	**Dew Point** Dew point sensor gives good accuracy.
ACETIC ACID	At 1% mass or below acetic acid nears the combined error threshold. At 3% mass acetic acid exceeds the error threshold. 100% acetic acid (glacial) is not recommended to be put into an instrument and can cause permanent damage to the sensors and surfaces. A thorough cleaning is recommended after running samples containing any concentration of acetic acid. B.P. 118 °C	**Concentration dependent** Dew point sensor gives good accuracy if acetic acid is kept at <1% by mass. If the mass percent acetic acid occasionally reaches several percent then a capacitance sensor may help. TDL is the only recommendation for nearly pure volatile compounds.

CITRIC ACID	Citric acid does not interfere with dew point sensors at concentrations up to 100%. M.P. 156 °C	**Dew Point** Dew point sensor gives good accuracy.
ETHANOL	At 1% mass or below ethanol nears the combined error threshold. At 3% mass ethanol exceeds the error threshold. B.P. 78 °C	**Concentration dependent** Dew point sensor gives good accuracy if ethanol is kept at <1% by mass. At concentrations of 1-5%, a capacitance sensor can be used occasionally. Prolonged exposure to ethanol risks poisoning the capacitance sensor causing irreversible drift, necessitating replacement of the sensor. At concentrations greater than 5% ethanol, a TDL is the only recommendation.
GLYCERIN	Glycerin does not interfere with dew point sensors at concentrations up to 100%. Vapor pressure of 0.003 mmHg at 50 ºC.	**Dew point**
ISOPROPANOL	At 1% mass or below isopropanol nears the combined error threshold. At 3% mass isopropanol exceeds the error threshold. B.P 83 °C	**Concentration dependent** Dew point sensor gives good accuracy if isopropanol is kept at <1% by mass. If the mass percent isopropanol occasionally reaches several percent then a capacitance sensor may help. TDL is the only recommendation for nearly pure volatile compounds.

MALIC ACID	Malic acid does not interfere with dew point sensors at concentrations up to 100%. M.P. 130 ºC	**Dew point**
PROPYLENE GLYCOL	Only above concentrations of 5% by mass does propylene glycol begin to interfere with a dew point sensor. B.P. 188 °C	**Concentration dependent** Dew point sensor gives good accuracy if propylene is kept at <3% by mass. If the mass percent propylene glycol occasionally reaches several percent then a capacitance sensor may help. TDL is the only recommendation for nearly pure volatile compounds.
LACTIC ACID	At concentrations up to 42.5% by mass lactic acid can be accurately read by a dew point sensor. 85% lactic acid is not recommended to be put into an instrument and can cause permanent damage to the sensors and surfaces. B.P. 122 °C	**Dew Point** Dew point sensor gives good accuracy up to concentrations of 42.5% by mass.
ESSENTIAL OILS		
CINNAMON OIL, STEAM DISTILLED *cinnamomum zeylanicum*	Dew point sensor reads 0.12 higher than TDL on average, well outside the acceptable range of accuracy. 90% cinnamaldehyde, B.P. 248 °C.[4]	**TDL** TDL is the only recommendation for nearly pure volatile compounds.
CLOVE OIL, STEAM DISTILLED *eugenia caryophyllata*	Contamination of dew point sensor. 45-90% of the essential oil is eugenol.[5]	**TDL** TDL is the only recommendation for nearly pure volatile compounds.
LEMON OIL, COLD PRESSED	Contamination of dew point sensor. Limonene (40%) and pinene (25%) dominant components.[12]	**TDL** TDL is the only recommendation for nearly pure volatile compounds.

PEPPERMINT OIL, STEAM DISTILLED *mentha piperita*	Contamination of dew point sensor. The main constituents are menthol (41%) and menthone (23%).[13]	**TDL** TDL is the only recommendation for nearly pure volatile compounds.
ROSEMARY OIL, STEAM DISTILLED *rosmarinus officinalis*	Depends highly on freshness of sample. Dew point sensor often reads consistently, but due to variability in samples may not always be reliable. Coffee contains numerous volatile compounds that vary in concentration with variety, roast, and sample handling.[15]	**TDL** TDL is the only recommendation for nearly pure volatile compounds.
COFFEE AND TEAS		
COFFEE	Contamination of dew point sensor. Major components are α-pinene and eucalyptol.[14]	**Highly variable** If you will be consistently measuring a wide variety of fresh coffee samples it is likely that a TDL will offer the greatest accuracy. If occasionally measuring coffee then a dew point sensor may suffice, but an instrument with a capacitance sensor will be more reliable.
SPICED BLACK TEA	Spiced teas often have essential oils added to the tea leaves which can cause interference with the dew point sensor.	**Variable** If you know you will be consistently measuring a wide variety of spiced tea samples it is likely that a TDL will offer the greatest accuracy. If occasionally measuring spiced teas then a dew point sensor may suffice, but an instrument with a capacitance sensor will be more reliable.
BLACK TEA	Tea leaves by themselves are able to be accurately measured with a dew point sensor.	**Dew point**
GREEN TEA	Tea leaves by themselves are able to be accurately measured with a dew point sensor.	**Dew point**

LEMON BLACK TEA	Spiced teas often have essential oils added to the tea leaves which can cause interference with the dew point sensor.	**Variable**
MINT BLACK TEA	Spiced teas often have essential oils added to the tea leaves which can cause interference with the dew point sensor.	**Variable**
EARLY GREY	Spiced teas often have essential oils added to the tea leaves which can cause interference with the dew point sensor.	**Variable**
CHICORY DRINK MIX	Chicory root extracts are known to contain many aroma compoundsand components with high volatility.[16]	**TDL**

† For the full data set, please request through your AQUALAB representative

Conclusions

Dried Spices and Herbs

The herbs and spices presented in this report fall into three categories regarding their performance: non-interfering, concentration dependent, and highly interfering. The spices and herbs measured for this report were not diluted in any way, and it's up to the end user to determine whether or not this represents their own samples.

Non-interfering: cayenne, medium chili, onion. A dew point sensor is best.

Concentration dependent: allspice, cinnamon, cumin, garlic, ginger, nutmeg, oregano, paprika, smoked paprika, white pepper. If using undiluted, a TDL is best, but at low concentrations a dew point sensor will work. **A capacitance sensor is a good compromise.**

Highly interfering: basil, black pepper, cloves, coriander, sage. **A TDL is the best way to reliably measure these herbs and spices unless they are significantly diluted.**

Essential Oils

Clove oil, peppermint oil, lemon oil, rosemary oil all had dew point sensors fail due to mirror contamination. Cinnamon oil was able to be measured in a dew point sensor, but it gave a reading significantly higher than the average TDL reading.

If you are looking to determine a_w of essential oils a TDL is the only reliable sensor given the low water content and high volatility of these mixtures.

Other Food Additives

The compounds presented in this report fall into two categories regarding their performance: non-interfering, and concentration dependent. There are numerous use cases for each of these components, and it's up to the end user to determine what instrument best suits their needs. For example, distilled white vinegar is typically 5% acetic acid and if you need to regularly determine the a_w for this type of sample, then you may need to consider a TDL. If you use samples containing diluted vinegar then a capacitance sensor may work well. If you know you have vinegar, but it's a small percentage of your sample then a dew point sensor may be sufficient.

Non-interfering: Ascorbic acid, citric acid, lactic acid, malic acid, glycerin.
A dewpoint sensor will work well for typical concentrations in food.

Concentration dependent: Acetic acid, ethanol, isopropanol, propylene glycol.
A TDL is the best instrument, but a capacitance sensor instrument may also be sufficient.

Coffee and Teas

Coffee is often problematic for a dew point sensor, but it is highly variable. There is variation from roast to roast and among varieties, but also between freshly ground vs. pre-packaged samples. If you are a coffee producer or roaster and are interested in determining the a_w of your product then the best choice is an instrument with a TDL sensor.

Teas can be accurately measured with a dew point sensor so long as they aren't flavored with highly volatile compounds, such as in some spiced teas. If you are a producer of spiced teas a TDL is necessary to accurately determine a_w in the presence of essential oils.

REFERENCES

1. Stewart, Toni-Moy; Lowe, Henry; Watson, Charah. Quantification and characterization of Pimenta dioica (Allspice) essential oil extracted via hydrodistillation,solvent and supercritical fluid extraction methodologies. *Am. J.of Essential Oils and Natural Products 2016, 4, 27-30.*

2. Janick, Jules. Basil: A Source of Aroma Compounds and a Popular Culinary and Ornamental Herb. *Perspectives on New Crops and New Uses* 1999, 499-505.

3. Stojanovic-Radic, Zorica. Piperine - A Major Principle of Black Pepper: A Review of Its Bioactivity and Studies. *Appl. Sci.* 2019, 9, 4270.

4. G. K. Jayaprakasha & L. Jagan Mohan Rao. Chemistry, Biogenesis, and Biological Activities of Cinnamomum zeylanicum. Critical Reviews in *Food Science and Nutrition* 2011, 51, 547-562.

5. Viljoen, Alvaro. Eugenol - From the Remote Maluku Islands to the International Market Place: A Review of a Remarkable and Versatile Molecule. *Molecules* 2012, 17, 6953-6981.

6. Mandal, Shyamapada, Coriander (Coriandrum sativum L.) essential oil: Chemistry and biological activity. *Asian Pac. J. Trop. Biomed.* 2015, 5, 421–428.

7. Jiang, Zi-Tao; Li, Rong. Chemical composition of the essential oil of Cumunum cyminum L. from China. *Flavor and Fragrance Journal 2004*, 19, 311-313.

8. An, Kejing; Wu, Jijun; Xu, Yujuan. Comparison of Different Drying Methods on Chinese Ginger (Zingiber Officinale Roscoe): Changes in Volatiles, Chemical Profile, Antioxidant Properties, and Microstructure. *J. Food Chem.* 2016, 197, 1292-1300.

9. Piras, Alessandra; Rosa, Antonella; Marongui, Bruno; Atzeri, Angela; Dessi, Assunta; Falconieri, Danilo; Porcedda, Silva. Extraction and Separation of Volatile and Fixed Oils from Seeds of Myristica fragrans by Supercritical CO2: Chemical Composition and Cytotoxic Activity on Caco - 2 Cancer Cells. J. Food Sci. 2012, 77, 448-453.

10. Marques, Antonio. Chemical composition and bioactivity of different oregano (Origanum vulgare) extracts and essential oil. *J. of the Sci. of Food and Ag.* 2013, 93, 2707-2714.

11. Andrea Böszörményi, Éva Héthelyi, Ágnes Farkas, Györgyi Horváth, Nóra Papp, Éva Lemberkovics, and Éva Szőke. Chemical and Genetic Relationships among Sage (Salvia officinalis L.) Cultivars and Judean Sage (Salvia judaica Boiss.) *J. of Ag. and Food Chem.* 2009, 57, 4663-4667.

12. Halima, Nihed. Citrus lemon essential oil: chemical composition, antioxidant and antimicrobial activities with its preservative effect against Listeria monocytogenes inoculated in minced beef meat. *Lipids in Health and Disease* 2017, 16, 146.

13. Schmidt, Erich. Chemical Composition, Olfactory Evaluation and Antioxidant Effects of Essential Oil from *Mentha x piperita. Nat. Prod. Comm.* 2009, 4, 1107-1112.

14. Carbonell-Barrachina, Angel. Composition of rosemary essential oil *(Rosmarinus officinalis)* as affected by drying method. *J. Food Eng.* 2010, 97, 253-260.

15. Ochiai N, Tsunokawa J, Sasamoto K, Hoffmann A. Multi-volatile method for aroma analysis using sequential dynamic headspace sampling with an application to brewed coffee. *J Chromatogr A*. 2014, 1371, 65-73.

16. Cadwallader, Keith; Wu, Tiandan. Identification of Characterizing Aroma Components of Roaster Chicory *"Coffee" Brews. J. of Ag. and Food Chemistry.* 2019, 67 (50), 13848-13859.

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