

Lavender Essential Oil

Chemistry in aqueous systems + compatibility hypothesis with low-pH electrolyzed water media

What this deck does (and does not) claim

It explains: (1) why essential oils do not have a meaningful “pH” on their own, (2) how they are stabilized at trace levels in water-based products, and (3) what must be tested to support compatibility with an acidic oxidizing electrolyzed-water medium. Compatibility is treated as a testable hypothesis, not an established fact.

“Stabilized pH” — what it means (and what it does not)

- pH is defined in terms of the activity of hydrogen ions in solution (an aqueous concept in standard practice).
- Lavender essential oil is a non-aqueous mixture (terpenes/terpenoids). As a separate oil phase, it does not have a meaningful pH value in the same sense as water-based solutions.
- When you see “pH of an essential-oil product,” it is the pH of the *continuous aqueous phase* (e.g., a spray, toner, or electrolyzed water), not of the oil molecules themselves.

Practical formulation translation:

- “Stabilized pH” usually means: (a) a buffered aqueous phase that stays within a target range over shelf life, and (b) compatible excipients (surfactants/solubilizers) whose performance is not degraded at that pH.
- For a fragrance/EO-in-water product, stability is dominated by: droplet size, solubilization mechanism, ionic strength/salinity, oxidation (air/light), and packaging — not by EO “pH.”

Key idea: pH is a property of the water-based medium; essential oils influence pH only indirectly (e.g., via additives, hydrolysis, oxidation).

Lavender EO chemistry: functional groups that control stability

Major constituents (typical; lot-dependent):

- Linalool (monoterpene alcohol) and linalyl acetate (monoterpene ester) are usually dominant in *Lavandula angustifolia* oils.
- Many lavender constituents are *unsaturated* (C=C bonds) and/or oxygenated (alcohols/esters) — key handles for oxidation and chlorination chemistry.
- Air exposure drives autoxidation of common fragrance terpenes; oxidation products can increase skin-sensitization risk and shift odor character.

Why this matters for electrolyzed-water media

If the aqueous medium contains strong oxidants (e.g., free chlorine as HOCl/Cl₂), reactive terpenes may be transformed, potentially reducing “lavender” actives and creating new products. The direction and magnitude depend on pH, oxidant dose, and how well the EO is physically shielded (e.g., micelles/encapsulation).

Aqueous stability depends on both chemistry (reactivity) and formulation physics (phase behavior).

Water-based products: dispersion and solubilization basics

Three regimes (increasing stability in water):

- Coarse dispersion (unstable): droplets separate over minutes–hours; typical when adding EO drops to water without a solubilizer.
- Emulsion / nanoemulsion (kinetically stable): oil-in-water droplets stabilized by surfactants; nanoemulsions often <200 nm and can appear translucent.
- Molecular encapsulation / inclusion: e.g., cyclodextrins reduce volatility and can “carry” terpene molecules in aqueous-compatible formats.

Why trace-level “ready-to-use” products can be stable:

- At very low EO loadings (ppm-to-low-%), properly chosen surfactant systems can keep droplets/micelles small and reduce separation.
- Physical stability (droplet size, Ostwald ripening, turbidity) is testable and often improves with optimized surfactant/co-solvent design.

Terminology: microemulsions are often thermodynamically stable; nanoemulsions are typically kinetically stable (require energy input to form).

Practical media options to disperse lavender EO to trace levels

Common scientific approaches (conceptual, not a recipe):

- Micellar solubilization: nonionic surfactants form micelles that “hide” oil molecules inside a hydrophobic core.
- Nanoemulsion route: high-shear mixing/sonication + surfactants creates small droplets; can improve clarity and stability.
- Microemulsion route: water + oil + surfactant + co-surfactant (often alcohols) can form single-phase systems in certain compositions.
- Cyclodextrin inclusion: terpene molecules (e.g., linalool) can form inclusion complexes that reduce volatility and improve handling in aqueous contexts.

Key constraints when the water phase is “non-plain water”

If the aqueous medium is strongly oxidizing (free chlorine/HOCl) and/or high-salinity, surfactant performance and EO stability can change. That is exactly why compatibility testing must cover both physical stability (phase behavior) and chemical stability (loss of terpene actives).

For diffusers: adding EO to water typically creates a coarse, unstable dispersion unless a purpose-designed solubilizer/emulsifier is used.

Choosing and holding a target pH in a diluted EO product

- pH selection is driven by the *medium's function* (skin contact vs hard-surface cleaning vs disinfection), plus chemical stability of the active system (e.g., free chlorine speciation).
- For chlorine-based oxidizing systems, pH strongly controls speciation (HOCl vs OCl⁻) and therefore antimicrobial activity; HOCl predominates in weakly acidic ranges.
- Buffers can stabilize pH but also add ionic strength and chemical "demand" that may consume oxidants or change surfactant behavior.

Two stabilization problems you must solve simultaneously:

- Physical stability: no phase separation, consistent droplet size, acceptable clarity/turbidity, no precipitation at the chosen salinity and pH.
- Chemical stability: key fragrance/active terpenes retained over time; oxidant strength (if used) retained within spec; minimal formation of unwanted byproducts.

In oxidizing media, "stable pH" is inseparable from "stable oxidant speciation" and "stable fragrance chemistry."

Electrolyzed-water dual streams (as described in your provided deck)

Acidic oxidizing stream (Anolyte)

- Typical parameters shown: pH 2–6.5 and ORP +900 to +1200 mV.
- Active reactive species listed: HO•, Cl₂, HCl, O₃, H₂O₂, HOCl.
- Your validation slides report an acidic stream measured at pH ~2.40 (UL stream).

Alkaline reducing stream (Catholyte)

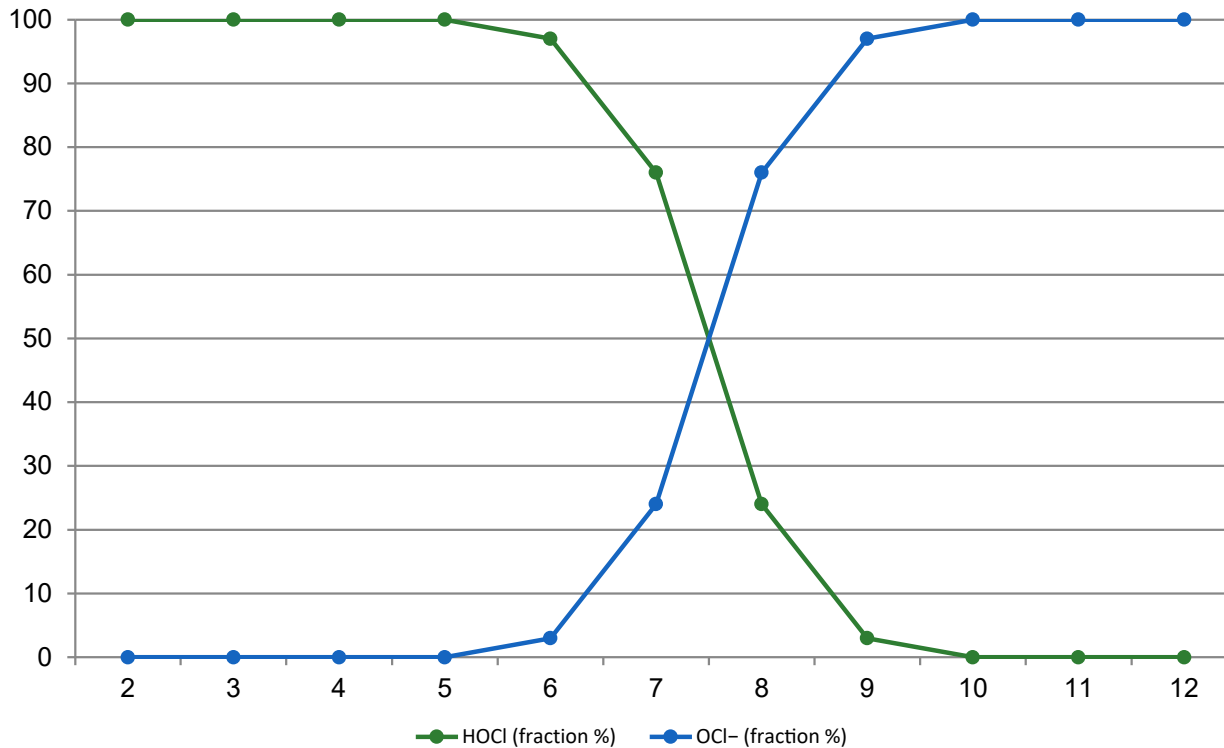
- Typical parameters shown: pH 7.4–12 and ORP around –850 (negative potential).
- Major species shown: NaOH, OH⁻, and H₂ (hydrogen evolution context).
- Your validation slides report an alkaline stream measured at pH ~11.55 (UH stream).

Scope note

You indicated that testing with the high-pH (alkaline) stream has not been explored yet. This deck focuses on the *low-pH oxidizing stream* as the candidate medium for a lavender-containing finished product.

Why low pH matters: HOCl vs OCl⁻ speciation is pH-controlled

Free chlorine equilibrium (simplified): $\text{HOCl} \rightleftharpoons \text{H}^+ + \text{OCl}^-$ (pKa \approx 7.5)



Interpretation

In weakly acidic ranges (roughly pH 3–6.5), HOCl dominates. At higher pH, OCl⁻ becomes dominant. If your low-pH stream is intended to deliver “active chlorine,” its speciation and stability are tightly linked to the maintained pH.

Important nuance

Below \sim pH 5, additional reactive chlorine species (e.g., dissolved Cl₂ or protonated species) can become relevant in some systems. This can change both efficacy and compatibility with organics.

Fractions computed from Henderson–Hasselbalch using pKa \approx 7.5 (illustrative).

Compatibility hypothesis: low-pH oxidizing medium as the water phase

Proposed target concept:

- Use the acidic oxidizing stream as the continuous aqueous medium for a finished, ready-to-use product.
- Incorporate lavender essential oil at trace levels (primarily for fragrance + secondary bioactivity), using a solubilization strategy that minimizes direct contact between reactive chlorine species and terpene molecules.
- Goal: preserve both functions — (a) oxidizing medium activity and (b) lavender's functional profile — over relevant shelf life and use conditions.

Scientific “must-be-true” conditions (operational definition of compatibility):

- Oxidant retention: free available chlorine (FAC) / ORP remains within target spec after adding EO + excipients.
- Terpene retention: key lavender markers (e.g., linalool/linalyl acetate) do not substantially degrade over the intended shelf life.
- No hazardous off-gassing or unacceptable byproduct formation under normal storage and use.
- Physical stability: clear or uniformly dispersed product with consistent dosing and no phase separation.

This slide defines “compatibility” as measurable retention of both oxidizing and lavender-EO functions.

Compatibility risks: oxidizing chlorine chemistry can transform terpenes

- Reactive chlorine species (HOCl and Cl₂) readily react with unsaturated organic compounds in air and on surfaces.
- Indoor-chemistry studies show HOCl/Cl₂ react with terpenes such as limonene, producing less volatile (often more oxygenated/chlorinated) products; this implies “terpene loss” is a plausible pathway in oxidizing media.
- By analogy (inference): many lavender terpenoids share reactive unsaturation; therefore, the low-pH oxidizing stream may reduce terpene actives unless they are sufficiently shielded or dosed very low.
- Any added organic load (EO, surfactants, solvents) can exert “chlorine demand,” lowering residual oxidant strength.

What failure could look like (chemistry indicators)

Rapid drop in FAC/ORP, color/odor drift, turbidity changes, and GC–MS showing loss of linalool/linalyl acetate or formation of new oxidation/chlorination products.

This is why a compatibility claim should be backed by analytical stability data (not just sensory impressions).

Suggested testing matrix to support (or falsify) compatibility

Design: compare “Analyte only” vs “EO only” vs “Analyte + EO formulation” across time.

A) Chemistry retention

- pH, ORP
- Free available chlorine (FAC)
- Headspace chlorine/off-odor
- GC–MS markers: linalool, linalyl acetate
- New byproducts screen

B) Physical stability

- Visual clarity/turbidity
- Droplet size (DLS) / microscopy
- Phase separation vs time
- Viscosity (if relevant)
- Container compatibility

C) Performance

- Odor profile over time
- Surface cleaning efficacy
- Microbial kill tests (if making disinfecting claims)
- Material compatibility (metals, plastics)
- User safety/irritation screening

Minimum “go/no-go” metrics (example):

- FAC retention: does the formulation keep oxidant within spec after fragrance addition?
- Terpene retention: do GC–MS markers remain within an acceptable window over shelf life?
- No significant chlorinated/irritant byproduct formation under typical use (screening dependent on claim).
- Stable dispersion/clarity with no separation across temperature cycling.

If any disinfecting/antimicrobial claims are made, ensure regulatory testing/label compliance for your jurisdiction.

Formulation strategies to improve coexistence (R&D directions)

1) Physical shielding

- Cyclodextrin inclusion complexes (linalool is a known CD guest): can reduce volatility and potentially reduce direct oxidant access.
- Micellar solubilization with nonionic surfactants: can compartmentalize EO molecules in hydrophobic cores; select excipients with oxidant tolerance.
- Nanoemulsions: small droplets reduce creaming; can be tuned for low EO load and controlled release.

Reality check

Shielding is not absolute: reactive oxidants may still diffuse into micelles/droplets. The question is whether the kinetics allow acceptable shelf life at the chosen EO dose.

2) Process & packaging tactics

- Point-of-use mixing (dual chamber or “add-on” fragrance cartridge) to avoid long-term contact between oxidants and terpenes.
- Minimize oxygen/light exposure to protect both HOCl and terpenes: opaque/UV-protective bottles, low headspace, compatible polymers.
- Use the lowest effective EO concentration (ppm-level fragrance can be perceptible), reducing oxidant demand and reaction probability.

Safety guardrail

Avoid uncontrolled gas release (chlorine/HOCl vapors). Validate headspace under heat/light stress. Ensure ventilation guidance for users and avoid pet exposure, especially cats.

Out of scope (for now): alkaline stream compatibility

- You noted that testing of the high-pH electrolyzed medium has not been explored at this time.
- From a chemistry standpoint, alkaline conditions can change surfactant behavior and can accelerate base-catalyzed transformations for some fragrance esters (potentially affecting odor), but the magnitude depends on pH and exposure time.
- If the alkaline stream is later considered, evaluate: ester stability, skin/material compatibility, and whether the “reducing/cleaning” role is intended to be separate (sequential use) or combined with fragrance.

Recommended next step

If/when you explore the alkaline stream, treat it as a new compatibility program (different chemistry, different failure modes). Start with a small scoping study before attempting a single “dual-function” combined product.

Key takeaways

- Essential oils do not have a meaningful pH by themselves; “pH” belongs to the aqueous medium (spray/analyte) and strongly controls oxidant speciation.
- Stabilizing lavender at trace levels in water requires formulation physics (micelles/emulsions/encapsulation) + chemical stability management (oxidation/chlorination).
- Your low-pH oxidizing stream is chemically powerful; compatibility with terpenes is plausible but non-trivial and must be demonstrated with retention testing (FAC/ORP + GC–MS markers).
- If coexistence is challenging, point-of-use mixing or encapsulation can reduce long-term oxidant–terpene contact while still providing fragrance and performance.

What we can build next

A slide deck section that translates the testing matrix into: (1) a draft product specification (pH, ORP/FAC, EO ppm target), (2) a small pilot stability protocol, and (3) acceptance criteria for “compatibility achieved.”

Selected references (non-exhaustive)

These sources support the *principles* in the deck. Formulation-specific compatibility requires your own analytical stability dataset.

- IUPAC Gold Book: pH definition (activity-based).
- Cherney (2006): free chlorine speciation; pKa ~7.5; low-pH potent oxidant discussion.
- Wang (2007 review): HOCl speciation and antimicrobial relevance; pH 3–6 HOCl predominance.
- Liu (2019) + Sambhakar (2023): nanoemulsion fundamentals; kinetic stability and preparation.
- Ciobanu (2012) + Rodríguez-López (2020): cyclodextrin inclusion with linalool/lavender EO.
- Wang et al. (2019) + Deeleepojananan et al. (2023): HOCl/Cl₂ reactions with terpenes (limonene) in indoor chemistry.
- Ishihara (2017): HOCl stability sensitivity to UV/air/temperature.
- User-provided AET/PBSWC deck (ADVANC~1.PDF): dual-stream pH/ORP/species and example measurements.

If you share your target FAC/ORP specs and intended use-case, we can tailor the stability protocol and acceptance criteria.