

PEER-REVIEWED AI SENSORY PUBLICATION | FOOD CHEMISTRY / FOOD QUAL PREFER

Predicting Temporal Dominance of Sensations (TDS) Kinetics from Instrumental GC-MS & Fast-GC Electronic Nose Profiles Using Recurrent Neural Networks (LSTM)

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EXECUTIVE ABSTRACT: Dynamic sensory profiling methods such as Temporal Dominance of Sensations (TDS) provide critical insights into temporal flavor release, dominance transitions, and lingering perception during mastication. However, human TDS panels require extensive screening, training under ISO 8586:2023, and repeated evaluations to reach statistical power. This research integrates fast-GC electronic nose headspace fingerprints and gas chromatography-mass spectrometry (GC-MS) volatile partition coefficients into a Bidirectional Long Short-Term Memory (Bi-LSTM) recurrent neural network. The neural model accurately predicts 60-second temporal dominance curves across 8 key sensory descriptors in carbonated beverages and emulsion systems ($R^2 = 0.914$, RMSE < 0.042) compared against 240 calibrated FIZZ Acquisition panel sessions.

KEY METHODOLOGICAL TAKEAWAYS & EMPIRICAL FINDINGS

01. Accurately maps volatile headspace fingerprints and Odor Activity Values (OAV) directly to 60-second millisecond-resolved human TDS dominance curves.
02. Incorporates bidirectional 2-layer LSTM with self-attention mechanism to balance immediate burst volatiles versus lingering retronasal flavor compounds.
03. Rigorously validated against 240 human sensory panel sessions conducted in ISO 8589 booths using FIZZ Acquisition TDS modules (temporal correlation $r = 0.914$, $p < 0.0001$).
04. Accelerates prototype dynamic flavor screening in RTD beverages and plant-based milks from 4 weeks of repetitive panel testing to under 15 minutes of in silico simulation.

1. THE ANALYTICAL CHALLENGE OF TIME-RESOLVED FLAVOR PERCEPTION

Dynamic sensory methods like Temporal Dominance of Sensations (TDS; Pineau et al., 2009) and Temporal Check-All-That-Apply (TCATA) capture the evolving sequence of dominant sensory attributes during food consumption. However, human TDS panels require extensive screening, training under ISO 8586:2023, and repeated evaluations to achieve statistical significance. Furthermore, rapid flavor volatile release often outpaces conventional static analytical testing.

Traditional static descriptive analysis (QDA) yields single intensity metrics that mask crucial temporal kinetics—such as sweetness delay, acidity burst, or lingering bitter off-notes. Capturing these temporal curves through human panels alone places significant logistical constraints on commercial product formulation.

2. MULTI-INSTRUMENTAL SENSING: GC-MS AND FAST-GC ELECTRONIC NOSE

Using an alpha-MOS Heracles Neo fast-GC electronic nose equipped with dual-column polarity (DB-5 non-polar and DB-1701 intermediate polarity) coupled to headspace solid-phase microextraction (SPME-GC-MS), volatile profiles were acquired across 140 carbonated beverage and plant-milk matrices.

Over 68 distinct volatile compounds were identified, with Odor Activity Values ($OAV = C_i / OT_i$) calculated against human olfactory thresholds. Gas-liquid partition coefficients (Henry's law constants and $\log K_{ow}$) were integrated to represent matrix retention and oral salivation release dynamics.

3. BIDIRECTIONAL LSTM NEURAL NETWORK ARCHITECTURE

A Bidirectional Long Short-Term Memory (Bi-LSTM) architecture was developed with an input dimension matching the 68 volatile OAVs and partition coefficients. Two stacked Bi-LSTM layers with 128 hidden units each, a recurrent dropout rate of 0.20, and a temporal self-attention mechanism were employed to assign adaptive weights across the mastication timecourse.

The output layer applies Softmax activation across 1-second discretizations over a 60-second mastication window, generating dominant probability trajectories across 8 sensory descriptors: Sweetness, Citric Acidity, Fruity Top-Note, Caramelized, Bitterness, Herbaceous, Creaminess, and Lingering Astringency.

4. VALIDATION AGAINST CALIBRATED FIZZ TDS PANELS

Predictions were benchmarked against empirical TDS data collected from 18 certified panelists in an ISO 8589 laboratory using FIZZ Network software. Chance and significance limits were computed according to Pineau et al. (2009).

The Bi-LSTM model predicted dominant attribute onset times with a mean absolute error of ± 1.4 seconds and peak dominance duration with an R^2 of 0.914 ($p < 0.0001$). Cross-validation across 240 industrial sensory sessions proved that the model generalizes robustly across variable sucrose-acid ratios and emulsified lipid contents.

5. FORMULATION APPLICATION AND R&D; EFFICIENCY

Integrating the trained neural network into formulation design allowed flavor chemists to simulate top-note modifications in silico. The AI identified that micro-encapsulating d-limonene in modified starch prolonged the citrus dominance window from 8.2s to 22.4s, eliminating a mid-palate flavor hollow without altering the total formulation cost.

By replacing manual bench iteration with predictive temporal simulation, commercial formulation teams reduced project turnaround from 4 weeks to under 15 minutes, establishing a digital twin for sensory dynamics.