Thermodynamic Equations of Nonequilibrium System for Measuring Odors by Gas Analyzers. Practical Example of a Microcontroller Calculation for Digital Odor Detection by Gas Analyzers

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***Abstract*— *A method for the digital measurement of odors using gas analyzers is presented. This capability enables a new level of precision in identifying spoiled products (e.g., in grain storage and transportation), detecting narcotics, digitizing odors in the culinary and cosmetics industries, and developing olfactory television. This paper details a measurement approach and methodology based on thermodynamic equations for a nonequilibrium odor measurement system. A practical example of a microcontroller calculation for a digital odor detection device using MQ-type gas analyzers is provided, including the process for determining the empirical coefficients integrated into the algorithm.*

Keywords*— *digital olfaction; electronic nose; gas sensor array; sensor fusion; microcontroller signal processing; odor profiling; grain spoilage detection.

I. INTRODUCTION

First, we must define what constitutes a measurable odor and how its digital detection can solve practical problems. An odor is manifested by the release of specific volatile organic compounds (VOCs) into the air. These VOC plumes, which form an odor's signature, propagate at characteristic speeds through a complex atmospheric environment. Their dispersion is influenced by factors including weight (molar mass), volume, temperature, humidity, incident light spectrum, air velocity, and other dynamic parameters that also affect biological olfactory receptors. While animals and humans use biological receptors to assess edibility or quality, digital odor detection provides an objective, quantifiable alternative. The application of odor analyzers allows for the determination of quality in products such as meat, fish, and grain. Specifically, this technology can identify the causes of spoilage in grain within elevators and shipholds, detect narcotics at security checkpoints in airports and customs, and has potential uses in creating odor-based multimedia and other fields.

II. PROBLEM FORMULATION

Commercial gas analyzers (e.g., MQ series) are calibrated to measure specific gases at set temperatures and concentrations. The resulting calibration curve for a target gas is stored in a microcontroller's memory. During operation, the device calculates and displays the measured concentration. The concentration of key VOCs that constitute a perceptible odor typically lies within the range of 10^{-4} to 10^{-5} ppm. While standard industrial gas analyzers can measure down to 10^{-3} ppm, specialized sensors approach the 10^{-4} ppm range, placing odor measurement at the limit of their detectable accuracy.

Critically, odor measurement is not a simple linear process but represents a **thermodynamically nonequilibrium measurement system** [1-5]. It must account for multiple interacting subsystems: the functional of odorant movement in air (E_1), the influence of the light spectrum (E_2), the influence of temperature and air humidity (E_3), the influence of air velocity (E_4), and the influence of the odor source mass (E_5). The methodology presented here involves determining experimental coefficients for these factors (E_1-E_5) and integrating them into a system of nonlinear thermodynamic equations for odor measurement within the microcontroller.

Odorous VOCs are predominantly hydrocarbons. Their movement in air is influenced by molecular structure and molar mass. Below are general characteristics of key hydrocarbon classes:

- **Alkanes (C_nH_{2n+2}):** sp^3-hybridization; tetrahedral geometry with bond angles of ~109.5°.
- **Alkenes (C_nH_{2n}):** sp^2-hybridization; trigonal planar geometry with bond angles of ~120°.
- **Alkynes (C_nH_{2n-2}):** sp-hybridization; linear geometry with bond angles of 180°.
- **Arenes (C_nH_{2n-6}):** sp^2-hybridization; planar geometry (e.g., benzene ring) with bond angles of 120°.

The empirical observation guiding sensor placement is as follows: A substance with a higher molar mass than air tends to settle faster. For example, the molar mass of air is approximately 28.97 g/mol. Opium ($C_{17}H_{19}NO_3$), amphetamine ($C_9H_{13}N$), and many nitrogen-containing compounds have higher molar masses. In practice, this means multi-sensor arrays for detecting such substances are often installed at a low height to sample air strata where heavier molecules may concentrate. Each target substance has characteristic differentials of propagation path (dS) and time (dT) in air, which form part of the calibration basis alongside the electrical differentials of the sensor (Conductivity dQ, Current dA, Resistance dR).

The core calculation in the microcontroller for one sensor channel integrates these concepts:

```
adc1 // Analog value from the detector

coefV = 0.1875 // Constant for ADC scaling

d = 1000 // Divider to obtain voltage

V = 5 // 5-volt detector power supply

Rload = 10000 // Load resistor value in Ohms

Ro = 122 // Sensor resistance in clean air under standard conditions
```

All data are processed within a system of equations modeling the nonequilibrium measurement system.

For detection, an array of different MQ-type gas sensors (Winsen Guangoyu) is used. Each sensor is calibrated for specific VOC profiles associated with a target odor. The microcontroller analyzes responses from all sensors, compares them to calibrated profiles, and provides a detection output for target substances at very low concentrations (10^{-4} – 10^{-5} ppm).

Examples of target substances and sensor configurations:

- **Heroin/Acetic Acid:** MQ-2, MQ-9 sensors.
- **Crack Cocaine/Burnt Rubber:** MQ-2, MQ-9 sensors.
- **Methamphetamine ($C_9H_{13}N$):** MQ-135, MQ-2, MQ-9 sensors.
- **Metformin/Fishy Odor:** MQ-135, MQ-2, MQ-9 sensors.

2.1 Thermodynamic Framework for a Nonequilibrium Odor Measurement System:

The measurement process is modeled using a thermodynamic framework for a system displaced from equilibrium. Let the system's state be defined by extensive parameters (E_i) and intensive parameters (P_i).

We introduce coefficient *A*, linking a change in an intensive parameter to changes in extensive parameters, and its reciprocal, the system capacity *K:*

$$K=1/A=dE/dP;A=1/K \tag{1}$$

The intensive parameters are functions of the extensive parameters:

$$P_1 = f_1(E_1, E_2, E_3, E_4, E_5); P_2 = f_2(E_1, E_2, E_3, E_4, E_5) \tag{2}$$

Differentiating these functions yields the system's response to changes in state:

$$dP_1 = A_{11}dE_1 + A_{12}dE_2 + A_{13}dE_3 + A_{14}dE_4 + A_{15}dE_5; dP_2 = A_{21}dE_1 + A_{22}dE_2 + A_{23}dE_3 + A_{24}dE_4 + A_{25}dE_5 \tag{3}$$

The state coefficients A_{ij} link changes in extensials (E_i) to changes in intensials (P_i). These coefficients are themselves functions of the system's state and change as the system moves from one nonequilibrium state to another. They represent the "quality" or structure of the measurement interaction, such as the functional of odor movement (E_1), light influence (E_2), etc.

The main and cross coefficients are functions of the extensive parameters:

$$A_{11} = f_{11}(E_1, E_2, E_3, E_4, E_5); A_{12} = f_{12}(E_1, E_2, E_3, E_4, E_5); A_{21} = f_{21}(E_1, E_2, E_3, E_4, E_5); A_{22} = f_{22}(E_1, E_2, E_3, E_4, E_5) \quad ....(4)$$

Differentiating these coefficients shows their dependence on the extensials:

$$\begin{aligned} dA_{11} &= B_{111}dE_1 + B_{112}dE_2 + B_{113}dE_3 + B_{114}dE_4 + B_{115}dE_5; dA_{12} \\ &= B_{121}dE_1 + B_{122}dE_2 + B_{123}dE_3 + B_{124}dE_4 + B_{125}dE_5; dA_{21} \\ &= B_{211}dE_1 + B_{212}dE_2 + B_{213}dE_3 + B_{214}dE_4 + B_{215}dE_5; dA_{22} \\ &= B_{221}dE_1 + B_{222}dE_2 + B_{223}dE_3 + B_{224}dE_4 + B_{225}dE_5 \end{aligned} \quad ...(5)$$

2.2 Microcontroller Implementation

The formalism above is implemented practically in the microcontroller algorithm. The core calculation for converting a raw sensor reading into an environmentally-corrected value uses the determined empirical coefficients (E_1-E_5).

The corrected sensor resistance (*Res_corrected*) is calculated as:

$$\text{Res\_corrected} = \frac{\text{Res}}{E_1 \times E_2 \times E_3 \times E_4 \times E_5} \quad (6)$$

where *Res* is the raw measured resistance of the sensor.

This corrected resistance is then used to calculate a target gas concentration (*p*), using a known atmospheric baseline (e.g., for CO_2):

$$p = \frac{\text{Res\_corrected}}{\text{ATM0\_GAS}} \quad (7)$$

Where:

- Res = detector resistance in Ohms (calculated from ADC).
- E_1 = odor movement functional coefficient.
- E_2 = light spectrum influence coefficient.
- E_3 = temperature & humidity influence coefficient.
- E_4 = air velocity influence coefficient.
- E_5 = odor source mass influence coefficient.
- adc0 = analog value from the detector.
- U = (adc0 * 0.1875) / 1000 = converted voltage.
- coefV = 0.1875 = ADC scaling constant.
- Res = (U * V - 1) * Rload = raw sensor resistance calculation (for a specific divider circuit).
- V = 5 = sensor supply voltage.
- Rload = load resistor value (e.g., 10 kΩ).
- p = calculated target gas concentration (ppm).
- ATM0_GAS = baseline atmospheric concentration of the target gas (e.g., 417.99 ppm for CO_2 in 2022).

III. RESULTS AND DISCUSSION

This approach was validated through practical experiments to determine the necessary empirical coefficients (E_1-E_5). Arrays of MQ gas analyzers (Winsen Guangoyu) were exposed to target odor sources under controlled variations: different distances, temperatures, humidity levels, wind speeds, light spectra, and source masses. Measurements were conducted within a controlled glass flask environment to isolate variables.

The work, conducted for the Greek-Ukrainian joint venture Harvard Marine LLC, led to the development of functional prototype "thermodynamic odor analyzers." The term "thermodynamic" reflects the use of the nonequilibrium system framework for calculation. Prototypes were built for:

1. Detecting specific narcotic substances.
2. Identifying grain spoilage via odors from bacteria, fungi, or pests.
3. Monitoring the onset of spoilage in meat and fish products in refrigerated retail displays.

These prototypes demonstrate the practical feasibility of the method, translating the theoretical framework into working devices for applied odor detection.

FIGURE 1: Prototype thermodynamic odor analyzers developed for various applications

IV. CONCLUSION

1) An approach and methodology based on thermodynamic equations for a nonequilibrium system have been developed for the digital measurement of odors using gas analyzers.
2) Thermodynamic equations for the digital odor detection system have been formulated. Experiments were conducted to determine the empirical coefficients (E_1-E_5) for a range of target odors, including narcotics, spoilage in grain, and spoilage in meat/fish products.
3) A practical example of the microcontroller calculation algorithm for a thermodynamic gas analyzer has been provided, demonstrating the integration of the empirical coefficients into the device's operational logic.

CONFLICT OF INTEREST

The authors declare no conflict of interest.

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