Transient Response Analysis for Temperature Modulated Chemoresistors

R. Gutierrez-Osuna$^{1,2}$, A. Gutierrez$^{1,2}$ and N. Powar$^2$

$^1$Texas A&M University, College Station, TX
$^2$Wright State University, Dayton, OH
Outline

- Introduction
  - Research objectives
  - Temperature modulation approaches

- Transient Response Analysis
  - Time-domain analysis
  - Time-constant or spectral analysis

- Pattern Analysis
  - Feature extraction
  - Performance measures

- Results
  - Experimental setup
  - Sensitivity and selectivity enhancements

- Concluding remarks
Objectives of this work

- Improve information content of COTS gas sensors by means of
  - **Instrumentation**: temperature modulation
  - **Computation**: transient-response analysis

- Evaluate various types of transient analysis techniques
  - Time-domain techniques
  - Time-constant-domain techniques
Outline

- Temperature modulation
  - Temperature oscillation
  - Temperature transients

- Transient analysis
  - Time domain
  - Time-constant domain

- Pattern analysis
  - Feature extraction
  - Performance measures

- Experimental validation
  - Experimental setup
  - Results
Temperature modulation

- **Basic principle**
  - Selectivity of metal-oxide chemoresistors depends on operating temperature
  - Capture the response of the sensor at multiple temperatures

from [Yamazoe and Miura, 1992]
Temperature modulation approaches

Temperature oscillation

- Sensor heater is driven by a continuous function
  - e.g., sine wave, ramp
- Information is in the quasi-stationary or dynamic response

Temperature transient

- Sensor heater is driven by a discontinuous function
  - e.g., step function, pulse
- Information is in the transient response
Temperature modulation examples

Temperature oscillation

Temperature transient

A AIR
B ACETONE
C AMMONIA
D IPA
E VINEGAR

S#4, 1-2V

W

M

AM

AIM

AI

IM

I

0.125Hz

x 10^{-4}

0 1 2 3 4 5

100 200 300 400 500 600 700 800

100 200 300 400

4 5 6 7 8 9
Transient response analysis

Objective

- Characterize the transient regime of a sensor to
  - Improve our understanding of the sensor’s behavior
  - Extract information to discriminate target analytes

How can the transient be characterized?

- Time domain
  - Extract parameters directly from the time samples
- “Frequency” domain
  - Convert the transient into a distribution of time constants

\[ f(t) = \int_0^\infty G(\tau)e^{-t/\tau} \, d\tau \]
Time vs. spectral representations
The Pade-Z Transform

- Pade-Z is a system-identification technique that finds a discrete multi-exponential model of the form

\[
f(t) = \sum_{m=1}^{M} G_m e^{-t / \tau_m}
\]

- Pade-Z in a nutshell
  - Compute the Z-transform of the sampled transient (at \(z_0\))
  - Fit a Pade approximant to the Z-transform
  - Compute the partial fraction expansion
  - Convert poles/residues into time-constants/amplitudes
  - Select a subset of the time-constants/amplitudes
Multi-Exponential Transient Spectroscopy

- METS is a signal-processing technique that yields a distribution or spectrum of time constants
  - A differentiation of the sensor transient in logarithmic-time scale

\[
METS_1(t) = \frac{d}{d(\ln t)} f(t) = \int_0^\infty \frac{t}{\tau} G(\tau) e^{-t/\tau} d\tau
\]

- METS is the convolution product of the true distribution with an asymmetric kernel

\[
h(y) = \exp(y - \exp(y)) \quad with \quad y = \ln(t)
\]
Ridge Regression Curve Fitting

- RRCF is statistical regression technique modified to produce a spectral representation of the transient
  - Based on the minimum mean-square error solution
    \[
    \{M, G_m, \tau_m\} = \arg\min_{M, G_m, \tau_m} \left[ \sum_{k=0}^{N-1} \left( f_k - \sum_{m=1}^{M} G_m e^{-kT / \tau_m} \right)^2 \right]
    \]

- Problems
  - The system of equations is non-linear in the time constants
  - M is unknown, meta-search is computationally intensive
  - Solution is ill-posed due to co-linearity

- Solutions
  - Pre-specify a fixed number of time constants
    \[
    \tau = \{0.01, 0.02, \ldots, 0.09, 0.1, 0.2, \ldots, 0.9, 1.2, \ldots, 9, \ldots\}
    \]
  - Stabilize the solution with a regularization term
**Validation on synthetic data**

- **Synthetic transient with three decays**
  - \( \tau_1 = 0.1 \text{ sec}, \ \tau_2 = 1 \text{ s}, \ \tau_3 = 10 \text{ s} \)
  - \( G_1 = -10, \ G_2 = +10, \ G_3 = -10 \)
  - DC offset \( G_0 = 10 \)
  - Gaussian noise \( N(\mu = 0, \sigma = 0.1) \)
FEATURE EXTRACTION
**Feature extraction**

- Features can be extracted from the sensor transient through window time slicing (WTS)
  - WTS can also be used in spectral representations
    - Interpretation as filter banks

![Sensor response graph](image)

![Spectrum graph](image)
Can the model parameters \( \{G_m, \tau_m\} \) be used as features?

- Partial fraction expansion is an ill-conditioned problem
- Small variations in the transient samples can lead to solutions with different number of exponentials

Conventional pattern-analysis techniques will expect a fixed dimensionality \( M \) for all examples
\textbf{Pade-Z feature extraction}

\textbf{Solution}

- Consider the Taylor-series expansion of $e^x$:

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots = \sum_{n=0}^{\infty} \frac{x^n}{n!}$$

- Re-grouping terms in the multi-exponential model:

$$\sum_{m=1}^{M} G_m e^{-t/\tau_m} = \cdots = \sum_{n=0}^{\infty} \frac{(-t)^n}{n!} \sum_{m=1}^{M} \frac{G_m}{\tau_m^n}$$

- Yields any desired (and fixed) number of features, regardless of the number of exponentials $M$ returned by Pade-Z

$$\left\{ \sum_{m=1}^{M} G_m, \sum_{m=1}^{M} \frac{G_m}{\tau_m}, \sum_{m=1}^{M} \frac{G_m}{\tau_m^2}, \sum_{m=1}^{M} \frac{G_m}{\tau_m^3}, \cdots \right\}$$
EXPERIMENTAL VALIDATION
Experimental setup

■ Sensor array
  • Four TGS Figaro sensors (2600, 2620, 2611, 2610)

■ Odor delivery
  • Static headspace analysis

■ Analyte database
  • Acetone (A), Isopropyl alcohol (I) and Ammonia (M)

■ Performance measures
  • Sensitivity and selectivity

■ Temperature profile
  • Staircase temperature modulation (STM)
Staircase temperature modulation

![Graphs showing temperature modulation for different gases](image-url)
**Feature sets**

- **Transient dataset**
  - Four sensors
  - Six transients per sensor
  - Four features per transient

- **Five feature sets**
  - WTS: 48 dimensions
  - Pade-Z: 48 dimensions
  - METS: 48 dimensions
  - RRCF: 48 dimensions
  - DC: 12 dimensions

- **Two datasets**
  - Sensitivity on serial dilutions
  - Selectivity on binary/ternary mixtures
**Rationale**

- Evaluate misclassification cost as a function of analyte concentration
  - Classification based on the nearest neighbor rule
- Misclassification cost
  - Penalize misclassifying analyte $X$ as analyte $Y$
  - Penalize misclassifying concentration $i$ as concentration $j$

\[
\text{Cost}(X_i|Y_j) = \frac{1}{\alpha} d(X,Y) + \frac{1}{\beta} d(i,j)
\]

where $d(i,j) = |i - j|$ and

\[
d(X,Y) = \begin{cases} 
0 & X = Y \\
1 & X \neq Y 
\end{cases}
\]
Sensitivity: results

- **Serial dilutions of individual analytes**
  - Base concentration (v/v)
    - A:10^{-4}\%, I:10^{-1}\%, M:1.0\%
    - These are near the DC-isothermal detection threshold
  - Dilutions
    - 5 levels with a 1/10 dilution factor
    - Distilled water is treated as a 6\textsuperscript{th} dilution level
  - Data collection
    - 17 samples per day
    - 4 days

![Graph showing sensitivity results](image_url)
Selectivity: performance measure

- **Rationale**
  - A good feature set will partition feature space into linearly separable odor-specific regions
  - For each analyte A, compute a linear discriminant function
    \[
    g_A(x) = \begin{cases} 
    1 & \text{if } x \in A \\
    0 & \text{otherwise} 
    \end{cases}
    \]
  - **Examples**
    - \( g_A(AB) = 1 \)
    - \( g_A(BC) = 0 \)
  - Discriminant functions are found with the Ho-Kashyap procedure
    - Guaranteed solution in the linearly separable case
    - Guaranteed convergence otherwise
Selectivity: results

- **Binary/ternary mixtures of analytes**
  - Base concentration (v/v)
    - A:0.3%, I:1.0%, M:33%
  - Equivalent analyte intensity on isothermal sensor response
- **Dilutions**
  - 3 levels with a 1/3 dilution factor
- **Data collection**
  - 24 samples per day
  - 3 days
CONCLUDING REMARKS
Conclusions

- Transient analysis
  - Time-domain vs. spectral characterization
  - Ridge Regression Curve Fitting

- Pattern analysis
  - Feature extraction
  - Performance measures

- Experimental results
  - Thermal transients provide improved sensitivity and selectivity
  - Thermal transients are faster; no need to reach S-S
  - Time-domain characterization provides a more compact code
Directions for future work

- **Data-driven placement of WTS kernels**
  - Kernels should be placed to maximize class separability

- **Improvements to Pade-Z characterization**
  - Regularization of partial fraction expansion
  - Development of classifiers for multi-modal densities

- **Experimental improvements**
  - Optimizing the duration of thermal transients
  - Comparison of ON/OFF and OFF/ON transients
  - Evaluation with micro hot-plates
QUESTIONS ...
THANK YOU