FROM RESEARCH TO INDUSTRY

cea tech

RECURSIVE LEAST SQUARES ALGORITHM DEDICATED TO EARLY RECOGNITION OF EXPLOSIVE COMPOUNDS THANKS TO MULTI-TECHNOLOGY SENSORS

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ICASSP 2013, VANCOUVER

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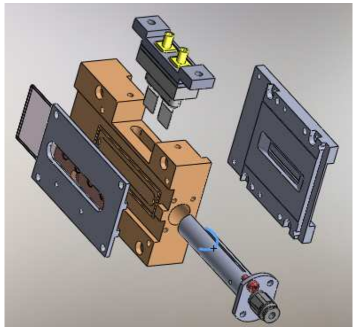

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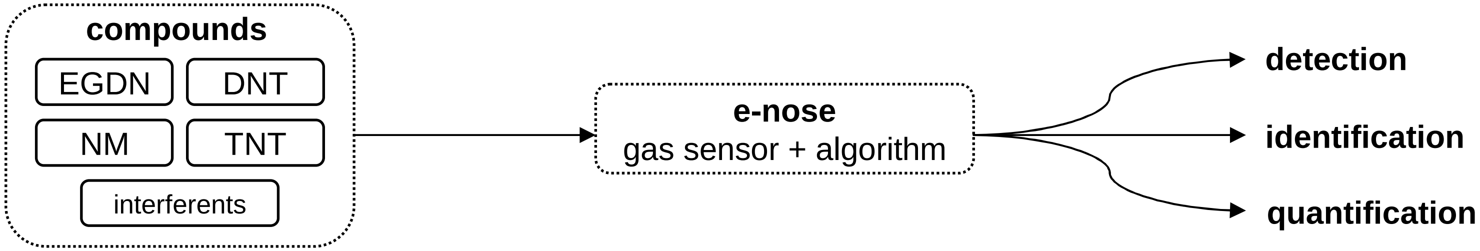
- **OVERVIEW**
  - Context
  - Prototype

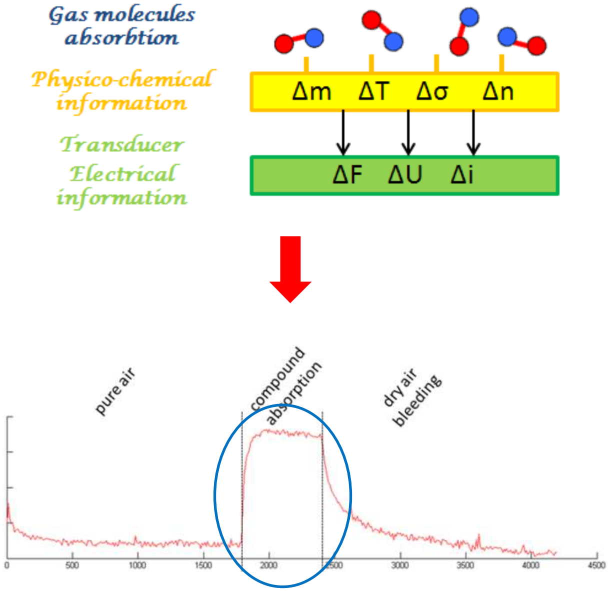
- **RECURSIVE LEAST SQUARES ALGORITHM**
  - Theorical basis & Principle
  - One dimensional signal case
  - Regularization
  - Multisensor adaptation

- **EXPERIMENTS**
  - Description
  - Results

CONTEXT

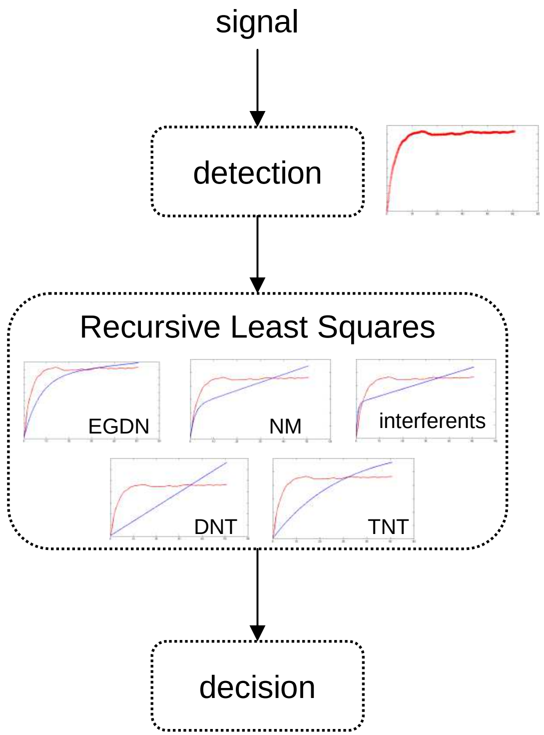


GAS SENSOR



- analyte
- sensitive material
- technology

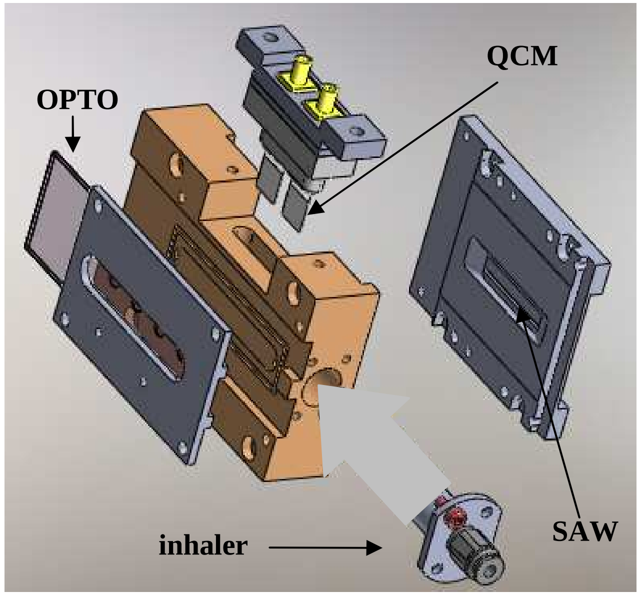
ALGORITHM

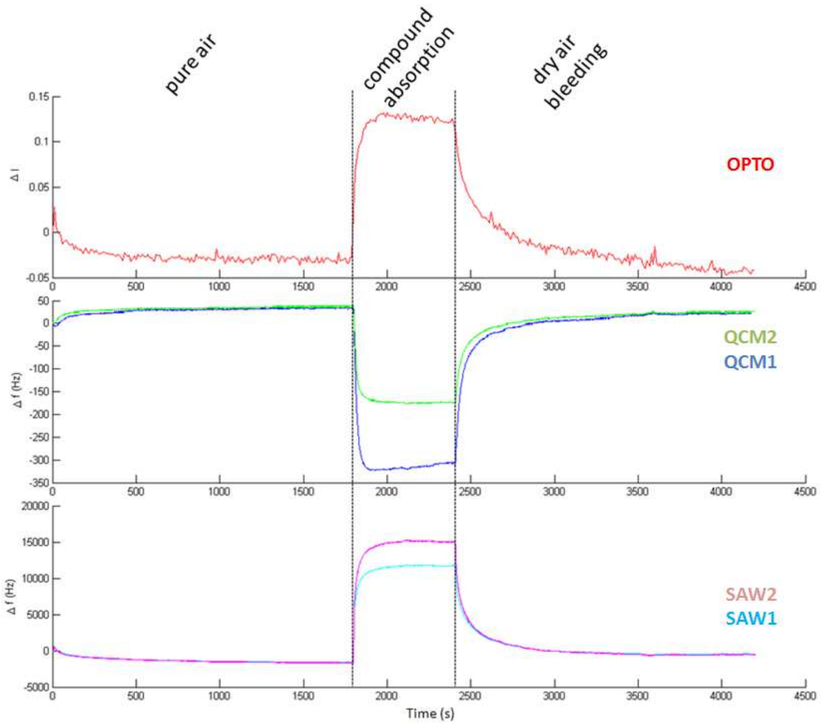


PROTOTYPE

Prototype based on a gas sensor array:

technology	active layers
Fluorescence (OPTO)	1
Quartz Crystal Microbalance (QCM)	2
Surface Acoustic Wave (SAW)	2

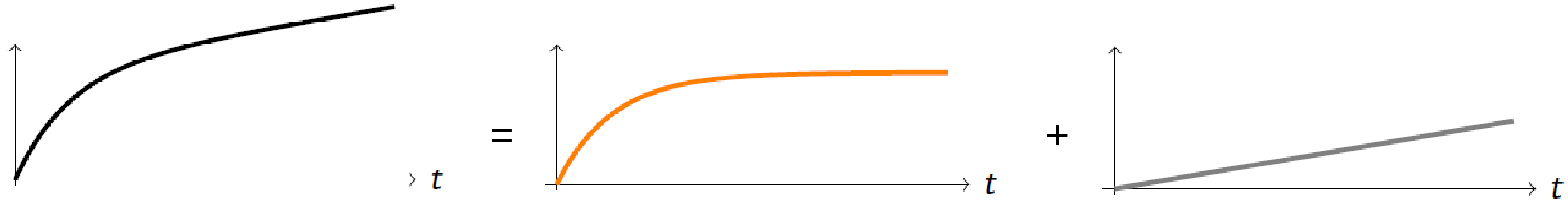




THEORICAL BASIS

first order response — linear drift

Langmuir model: $$f_{\tau,\delta}(t, Q, \alpha, \beta) = \underbrace{Q.\delta.\left(1 - e^{-t/\tau}\right)}_{\text{first order response}} + \underbrace{\alpha.t + \beta}_{\text{linear drift}}$$



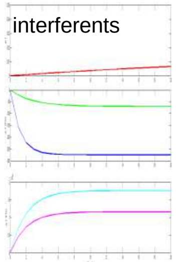
used to build models

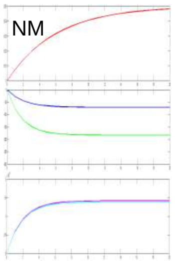
- parameters depending on the absorption affinity between the unknown gas and the sensor:
  - τ time constant
  - δ sensitivity

estimated by RLS algorithm

- parameters depending on experimental conditions:
  - Q concentration of the compound
  - α slope of the sensor linear drift
  - β sensor offset

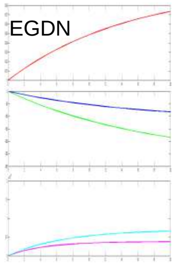
PRINCIPLE

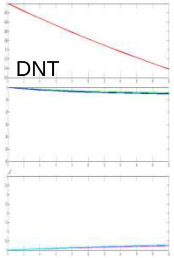


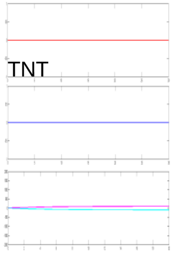


$(\tau^{(c)}, \delta^{(c)})$

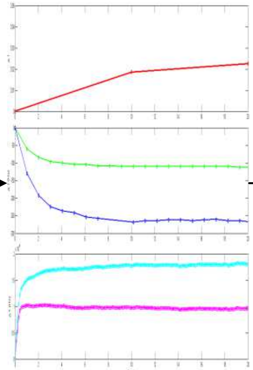
are set using training examples to build models



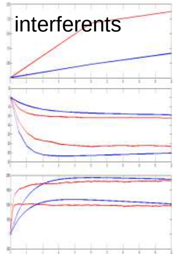


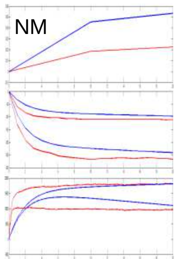


MODELS



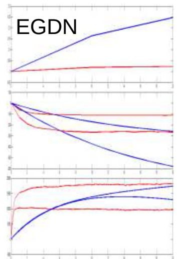
ACQUISITION

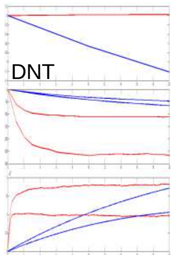


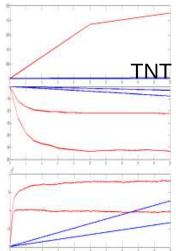


$(Q^{(c)}, \alpha^{(c)}, \beta^{(c)})$

are estimated in such a way each model best fits the real data







RECURSIVE LEAST SQARES

DECISION

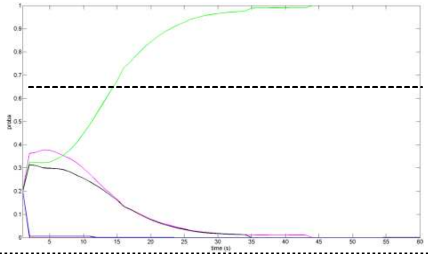
e_{DNT} → P_{DNT}

e_{TNT} → P_{TNT}

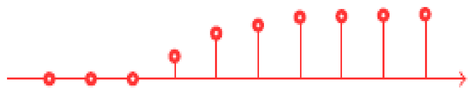
e_{EGDN} → P_{EGDN}

e_{NM} → P_{NM}

$e_{interferents}$ → $P_{interferents}$



RLS: ONE DIMENSIONAL SIGNAL CASE



Least Squares:

$$Z = H\theta + E$$

$$= \begin{pmatrix} & \mathrm{M} & \\ \delta(1 - e^{-\frac{t}{\tau}}) & t & 1 \\ & \mathrm{M} & \end{pmatrix} \begin{pmatrix} Q \\ \alpha \\ \beta \end{pmatrix} + E$$

- Z acquisition vector
- H model matrix
- θ vector of parameters
- E error

Pseudo-inverse solution: $\hat{\theta} = (H^T H)^{-1} H^T Z$

Recursive Least Squares:

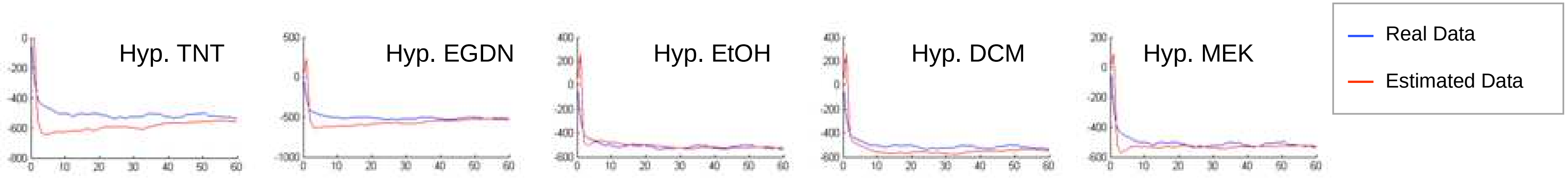
$$\begin{pmatrix} Z_k \\ z_{k+1} \end{pmatrix} = \begin{pmatrix} H_k \\ h_{k+1} \end{pmatrix} \theta + \begin{pmatrix} E_k \\ \varepsilon_{k+1} \end{pmatrix}$$

$$\Leftrightarrow Z_{k+1} = H_{k+1}\,\theta + E_{k+1}$$

Solution: $\hat{\theta}_{k+1} = \hat{\theta}_k + P_{k+1} h_{k+1}^T (z_{k+1} - h_{k+1}\hat{\theta}_k)$ with $P_{k+1} = P_k - \dfrac{P_k h_{k+1}^T h_{k+1} P_k}{1 + h_{k+1}^T P_k h_{k+1}}$ | $\hat{\theta}_0 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$, $P_0 = Id$

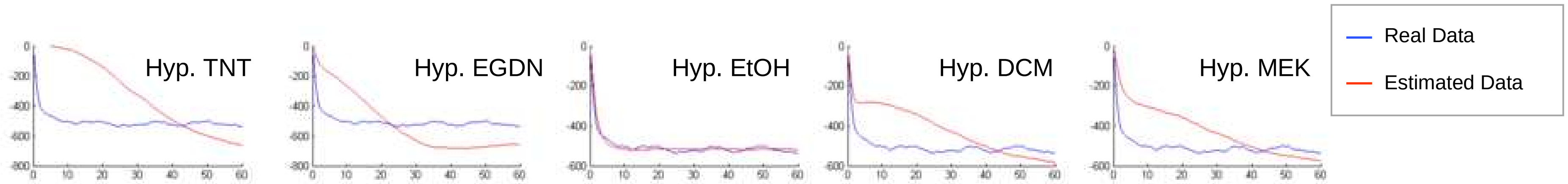
RLS: REGULARIZATION

Q, α and β can freely evolve: the sensor drift and the exponential part cannot be discriminated correctly



<u>*Reguralization*</u>: $$\hat{\theta} = \arg\min_{\theta} \left(\|H\theta - Z\|^2 + \|\Gamma\theta\|^2 \right)$$ with $$\Gamma = \begin{pmatrix} \Gamma_Q & 0 & 0 \\ 0 & \Gamma_\alpha & 0 \\ 0 & 0 & \Gamma_\beta \end{pmatrix}$$

Γ_Q, Γ_α and Γ_β are used to set each parameter inertial.



Solution: $$\hat{\theta}_{k+1} = \hat{\theta}_k + P_{k+1} h_{k+1}^T (z_{k+1} - h_{k+1}\hat{\theta}_k)$$ with $$P_{k+1} = P_k - \frac{P_k h_{k+1}^T h_{k+1} P_k}{1 + h_{k+1}^T P_k h_{k+1}}$$

$$\hat{\theta}_0 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

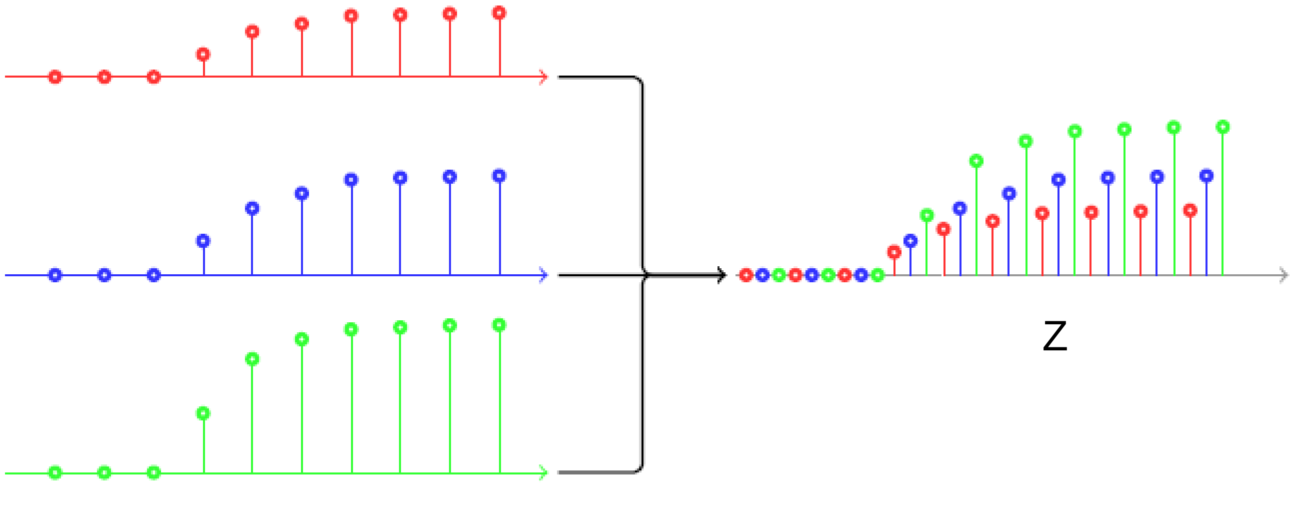
$$P_0 = (\Gamma^T \Gamma)^{-1}$$

RLS: MULTISENSOR CASE

$$Z^1 = \begin{pmatrix} & \vdots & \\ \delta_1(1-e^{-\frac{t}{\tau_1}}) & t & 1 \\ & \vdots & \end{pmatrix} \begin{pmatrix} Q \\ \alpha_1 \\ \beta_1 \end{pmatrix} + E^1$$

$$Z^2 = \begin{pmatrix} & \vdots & \\ \delta_2(1-e^{-\frac{t}{\tau_2}}) & t & 1 \\ & \vdots & \end{pmatrix} \begin{pmatrix} Q \\ \alpha_2 \\ \beta_2 \end{pmatrix} + E^2$$

$$Z^3 = \begin{pmatrix} & \vdots & \\ \delta_3(1-e^{-\frac{t}{\tau_3}}) & t & 1 \\ & \vdots & \end{pmatrix} \begin{pmatrix} Q \\ \alpha_3 \\ \beta_3 \end{pmatrix} + E^3$$



$$Z = \begin{pmatrix} & & & \vdots & & & \\ \delta_1(1-e^{-\frac{t}{\tau_1}}) & t & 0 & 0 & 1 & 0 & 0 \\ & & & \vdots & & & \end{pmatrix} \begin{pmatrix} Q \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix} + E$$

RLS: MULTISENSOR CASE

$$Z^1 = \begin{pmatrix} & \vdots & \\ \delta_1(1-e^{-\frac{t}{\tau_1}}) & t & 1 \\ & \vdots & \end{pmatrix} \begin{pmatrix} Q \\ \alpha_1 \\ \beta_1 \end{pmatrix} + E^1$$

$$Z^2 = \begin{pmatrix} & \vdots & \\ \delta_2(1-e^{-\frac{t}{\tau_2}}) & t & 1 \\ & \vdots & \end{pmatrix} \begin{pmatrix} Q \\ \alpha_2 \\ \beta_2 \end{pmatrix} + E^2$$

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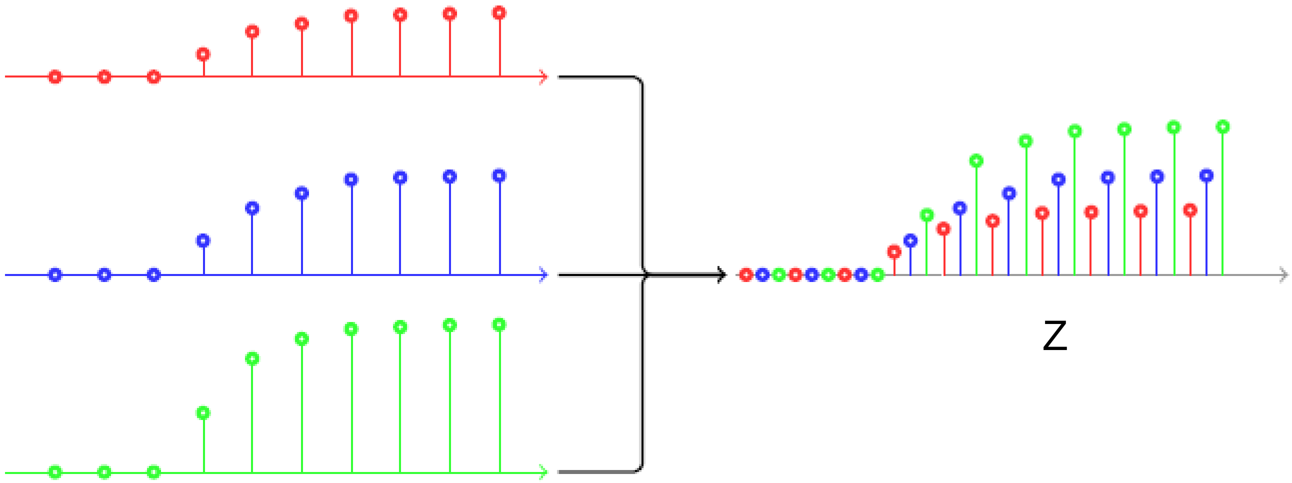


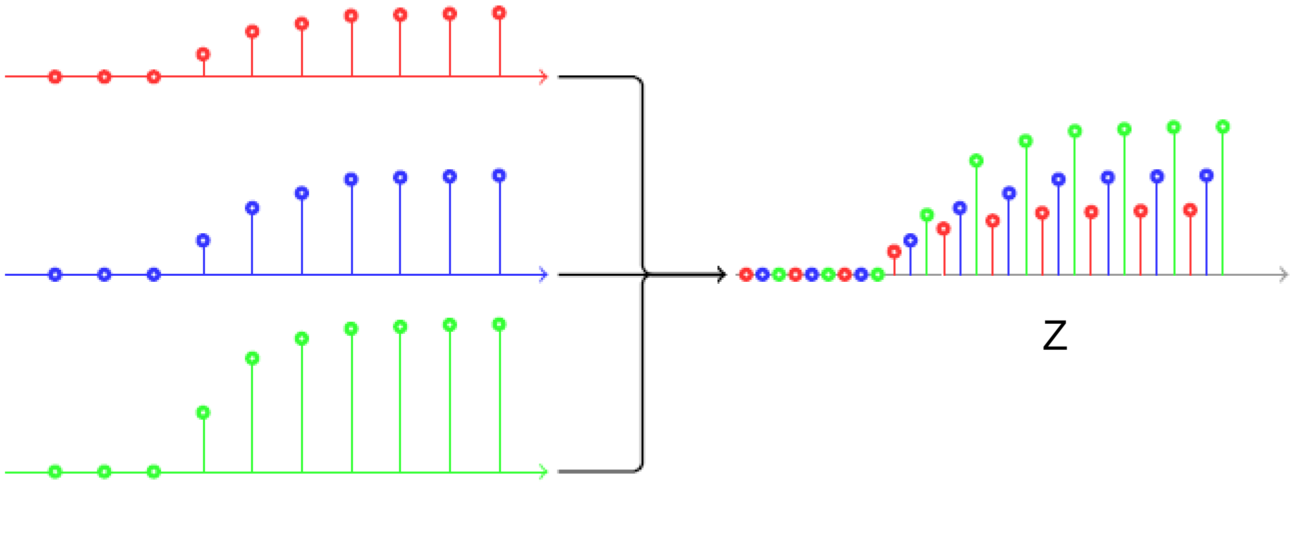
$$Z = \begin{pmatrix} & & & \vdots & & & \\ \delta_2(1-e^{-\frac{t}{\tau_2}}) & 0 & t & 0 & 0 & 1 & 0 \\ & & & \vdots & & & \end{pmatrix} \begin{pmatrix} Q \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix} + E$$

RLS: MULTISENSOR CASE

$$Z^1 = \begin{pmatrix} & \vdots & \\ \delta_1(1-e^{-\frac{t}{\tau_1}}) & t & 1 \\ & \vdots & \end{pmatrix} \begin{pmatrix} Q \\ \alpha_1 \\ \beta_1 \end{pmatrix} + E^1$$

$$Z^2 = \begin{pmatrix} & \vdots & \\ \delta_2(1-e^{-\frac{t}{\tau_2}}) & t & 1 \\ & \vdots & \end{pmatrix} \begin{pmatrix} Q \\ \alpha_2 \\ \beta_2 \end{pmatrix} + E^2$$

$$Z^3 = \begin{pmatrix} & \vdots & \\ \delta_3(1-e^{-\frac{t}{\tau_3}}) & t & 1 \\ & \vdots & \end{pmatrix} \begin{pmatrix} Q \\ \alpha_3 \\ \beta_3 \end{pmatrix} + E^3$$

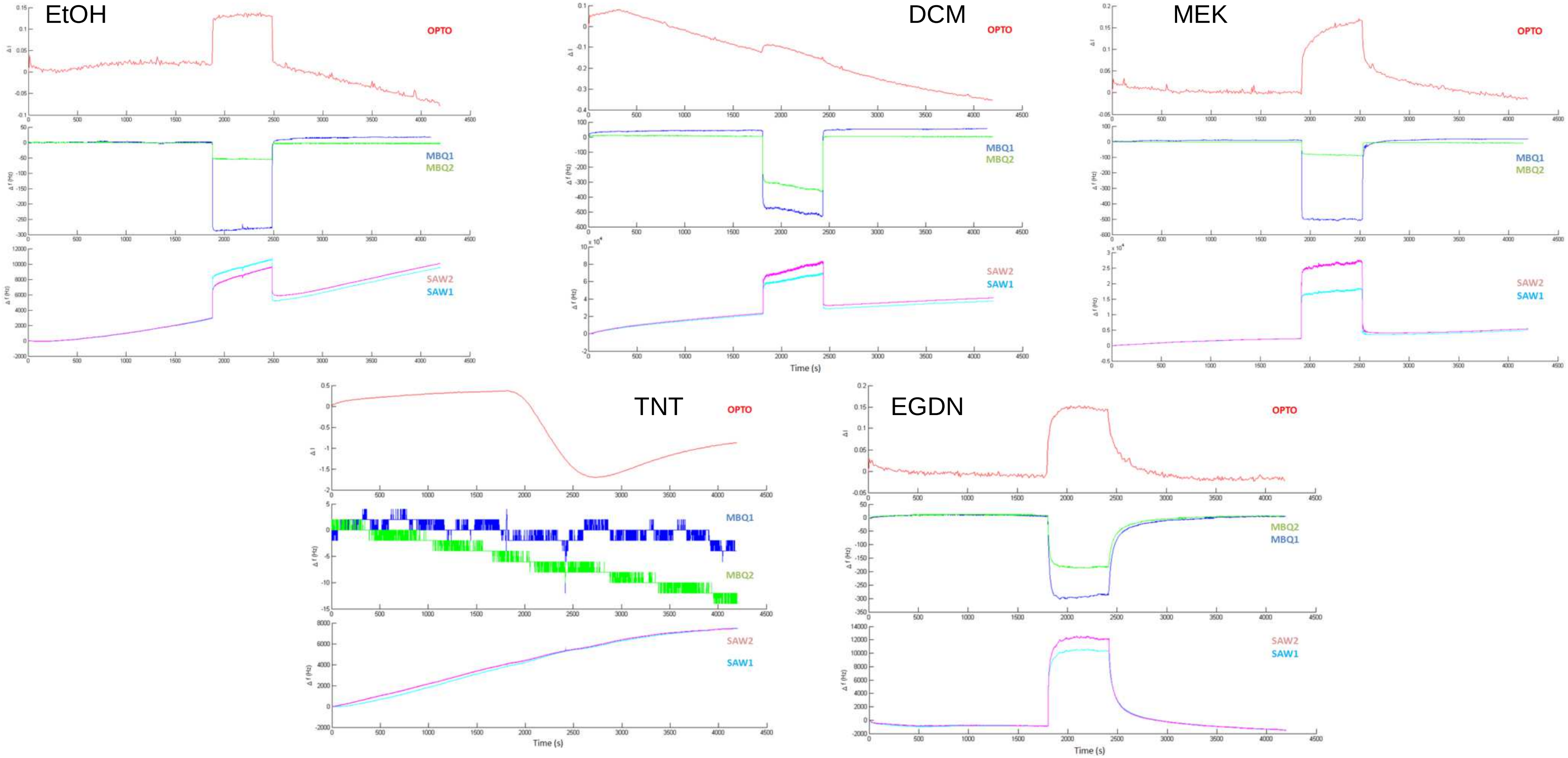


$$Z = \begin{pmatrix} & & & \vdots & & & \\ \delta_3(1-e^{-\frac{t}{\tau_3}}) & 0 & 0 & t & 0 & 0 & 1 \\ & & & \vdots & & & \end{pmatrix} \begin{pmatrix} Q \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix} + E$$

- work in real time
- process samples from sensors with different sampling frequencies
- discriminate compounds with different kinetics and/or amplitude ratio from the multi-sensor

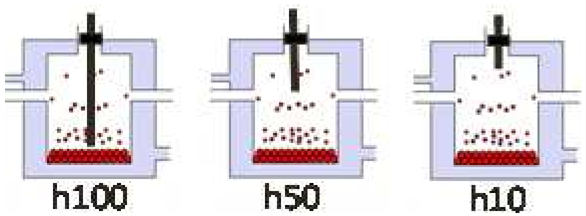
EXPERIMENTS: DESCRIPTION

Compounds:



Protocol:

- lab condition
- vapour generation cell
- different concentrations



Training set: only h100 acquisitions

Test set: h100, h50 and h10 acquisitions

EXPERIMENTS: RESULTS

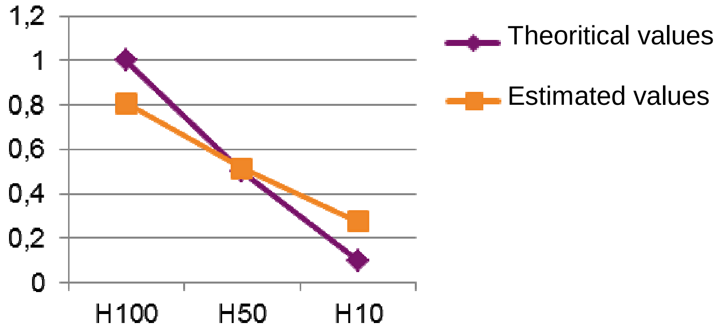
1) Identification rate:

Explosives	TNT			EGDN		
Concentration	h100	h50	h10	h100	h50	h10
Identification rate	3/3	3/3	3/3	3/3	3/3	3/3
Identification time (s)	47	43	47	31	32	32
Interferents	**EtOH**			**DCM**	**MEK**	
Concentration	h100	h50	h10	h100	h100	
Identification rate	3/3	3/3	2/3	2/3	3/3	
Identification time (s)	35	32	31	31	34	

2) Identification rate:

Explosives	TNT			EGDN		
Concentration	h100	h50	h10	h100	h50	h10
QCM+SAW	0/3	0/3	0/3	3/3	3/3	3/3
OPTO+SAW	3/3	3/3	3/3	3/3	2/3	0/3
OPTO+QCM	3/3	3/3	3/3	3/3	2/3	1/3
Interferents	**EtOH**			**DCM**	**MEK**	
Concentration	h100	h50	h10	h100	h100	
QCM+SAW	3/3	3/3	2/3	2/3	3/3	
OPTO+SAW	2/3	3/3	2/3	2/3	1/3	
OPTO+QCM	1/3	1/3	2/3	2/3	0/3	

Quantification:



- identification rate: 94%
- identification time < 60s
- robustness to variations of concentration

- performances are deteriorated when a technology is missing

Video

TNT, EGDN vs. EtOH, DCM, MEK

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