Discrimination of gas-phase emissions from building material samples by combining two gas-sensor arrays
Objective

→ Objective: assessment of the a priori discrimination power of a merged system integrating 2 different gas sensor arrays to emissions of 20 building materials.

→ Part of the European project SysPAQ (Müller et al., 2008, presented at Indoor Air 2008, paper id 530)

→ Experiments were performed by AlphaMOS using 24 individual metal oxide sensors and FZK-IMT using the Kamina chip of 38 sensor segments (details presented in Goschnick et al., Indoor Air 2008, paper id 259)

→ Building material samples were provided by DTU and SBi from Denmark.
Selection of signal feature: 3 different features tested, relative change in resistance $\Delta R/R$, resistance change rate $dR/dt$ and time to reach maximum signal change $t_{max}$ to improve discrimination.
Selection of optimal profile → time at maximum inter-sensor variance

Construction of several data matrixes using the signal features for the 2 sensor arrays and the merged system.
Multivariate statistical analysis

For each data matrix, we perform the following:

→ Principal component analysis

→ Hierarchical classification on all dimensions

→ Automatic selection of the 3 best partitions.

→ Best discrimination is achieved for

$$\frac{\text{Inertia}_\text{inter-classes}}{\max(\text{Inertia}_\text{intra-classes})} \quad \text{maximum}$$

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Results

Array 1
38 sensor
Segments
\( \Delta R/R \)

Array 2
24 individual
sensors
\( \Delta R/R \)

7 classes
Ratio = 30

4 classes
Ratio = 17

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Results

<table>
<thead>
<tr>
<th>Sensor array 1</th>
<th>Sensor array 2</th>
<th>Number of classes</th>
<th>I inter-classes / I total</th>
<th>I total</th>
<th>Max I intraclass</th>
<th>I inter / I intra ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta R/R_0$ (max var)</td>
<td>$\Delta R/R_0$ (max var)</td>
<td>9</td>
<td>0.88</td>
<td>60</td>
<td>1.78</td>
<td>30</td>
</tr>
<tr>
<td>$\Delta R/R_0$ (max var)</td>
<td>$\Delta R/R_0$ (max var)</td>
<td>7</td>
<td>0.92</td>
<td>36</td>
<td>1.09</td>
<td>30</td>
</tr>
<tr>
<td>$\Delta R/R_0$ (max var)</td>
<td>$\Delta R/R_0 + dR/dt + t_{95}$</td>
<td>4</td>
<td>0.84</td>
<td>24</td>
<td>1.17</td>
<td>17</td>
</tr>
<tr>
<td>$\Delta R/R_0 + dR/dt + t_{max}$</td>
<td>$t_{95}$</td>
<td>10</td>
<td>0.84</td>
<td>108</td>
<td>6.33</td>
<td>14</td>
</tr>
<tr>
<td>$dR/dt$ (max var)</td>
<td></td>
<td>7</td>
<td>0.83</td>
<td>36</td>
<td>2.19</td>
<td>14</td>
</tr>
<tr>
<td>$t_{max}$</td>
<td></td>
<td>5</td>
<td>0.78</td>
<td>71</td>
<td>4.96</td>
<td>11</td>
</tr>
<tr>
<td>$\Delta R/R_0 + dR/dt + t_{max}$</td>
<td>$dR/dt$ (max var)</td>
<td>5</td>
<td>0.83</td>
<td>23</td>
<td>2.21</td>
<td>9</td>
</tr>
<tr>
<td>$\Delta R/R_0 + dR/dt + t_{max}$</td>
<td>$\Delta R/R_0 + dR/dt + t_{95}$</td>
<td>5</td>
<td>0.73</td>
<td>24</td>
<td>2.24</td>
<td>8</td>
</tr>
<tr>
<td>$\Delta R/R_0 + dR/dt + t_{max}$</td>
<td>$\Delta R/R_0 + dR/dt + t_{95}$</td>
<td>5</td>
<td>0.56</td>
<td>179</td>
<td>25.50</td>
<td>4</td>
</tr>
</tbody>
</table>

→ Best discrimination is achieved when merging relative change in resistances from the two sensor arrays.
Best discrimination

9 classes
Ratio = 30

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• According to the extracted feature, different \textit{a priori} classifications of building materials can be achieved by sensor arrays.

• Data merging does not automatically improve discrimination.

• This study presents a method to optimize discrimination and get homogeneous classes. Classes gather materials that share a common feature in the response of sensors.

• But in order to relate it to perceived air quality, the olfactory differences between samples need first to be assessed, e.g. \textit{a priori} classification of building material based on reliable olfactory information.