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APPLICATION OF MACHINE LEARNING METHODS FOR ANALYZING DATA FROM SEMICONDUCTOR GAS SENSORS IN DYNAMIC TEMPERATURE MODE*

Igor Isaev[1,2,3], Kirill Chernov[4], Nickolay Shchurov[1,4], Sergey Dolenko[1], and Valeriy Krivetskiy[3,5]

[1] D.V. Skobeltsyn Institute of Nuclear Physics, MSU, Moscow, Russia.
[2] Kotelnikov Institute of Radio Engineering and Electronics, RAS, Moscow, Russia.
[3] Scientific-Manufacturing Complex Technological Centre, Zelenograd, Moscow, Russia
[4] Physics Department, MSU, Moscow, Russia
[5] Chemistry Department, MSU, Moscow, Russia

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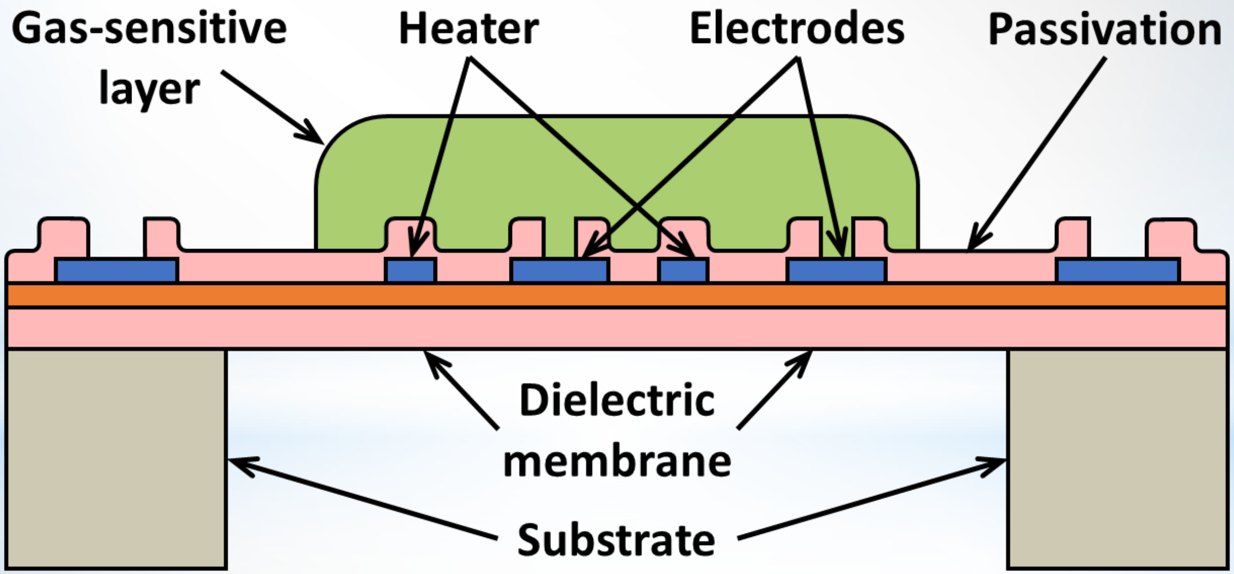
Physical experiment

Gas sensor

Schematic design of a semiconductor gas sensor

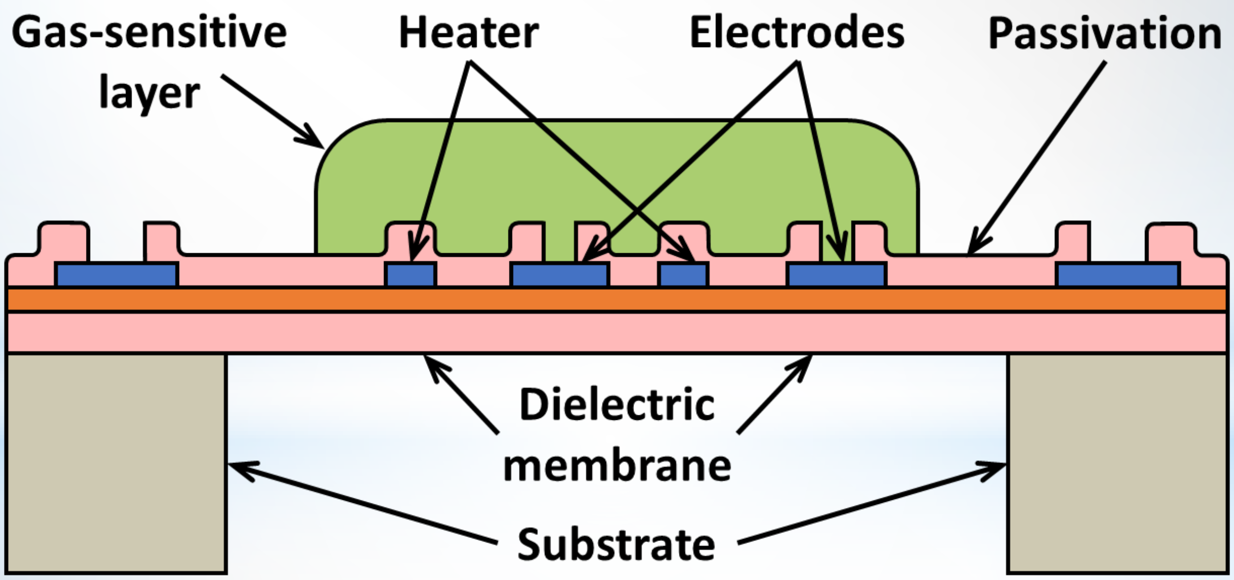


The principle of operation of the sensor is based on the fact that gas molecules binding to the sensor material affect its conductivity (electrical resistance).

Physical experiment

Gas sensor

Schematic design of semiconductor gas sensor



Binding degree depends on:

- ❑ Type of gas and its concentration
- ❑ Sensor material
- ❑ Temperature

Physical experiment

Gas sensor

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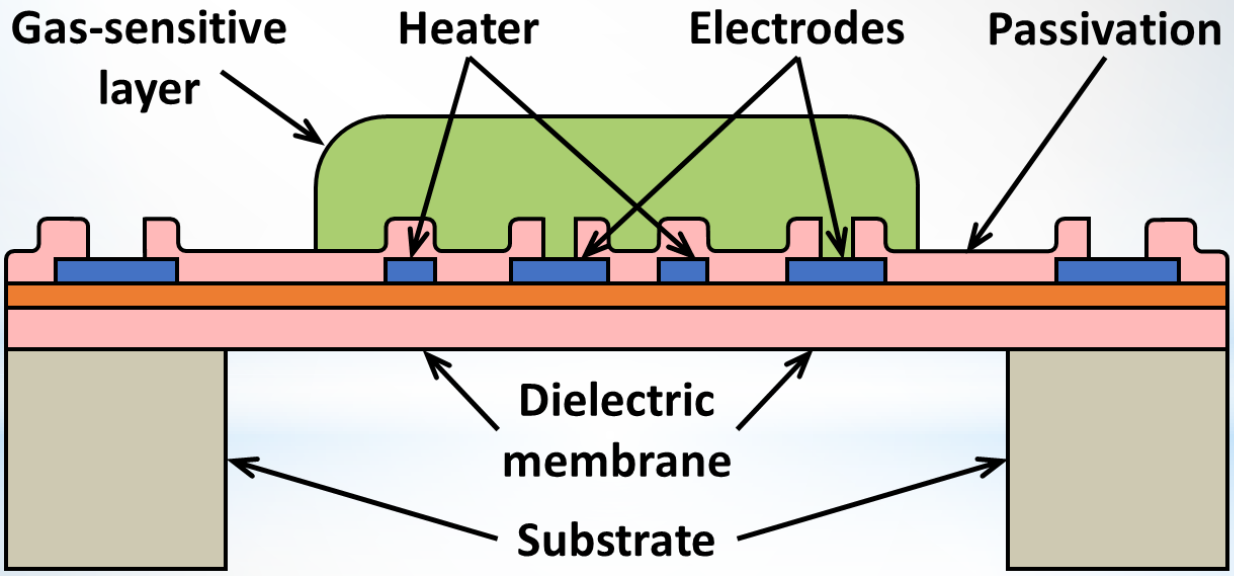

Binding degree depends on:

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- ❑ Sensor material
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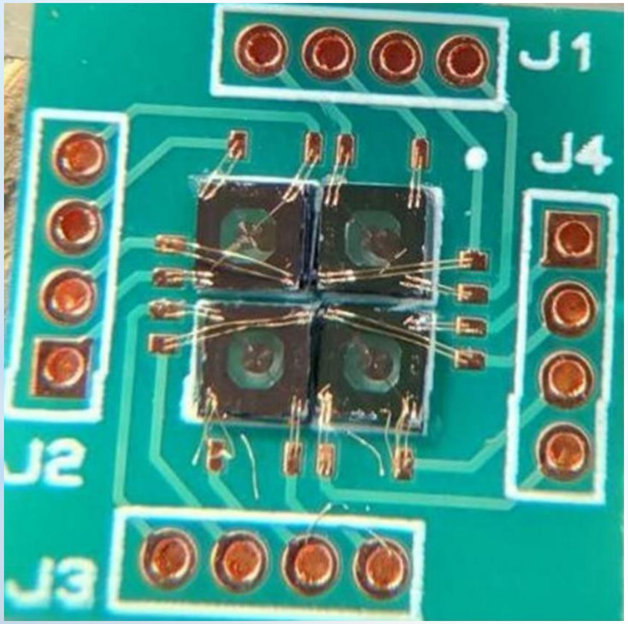
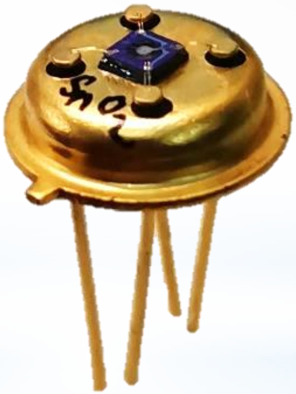
Set of semiconductor sensors with different doping components are used to achieve selectivity when detecting certain gases

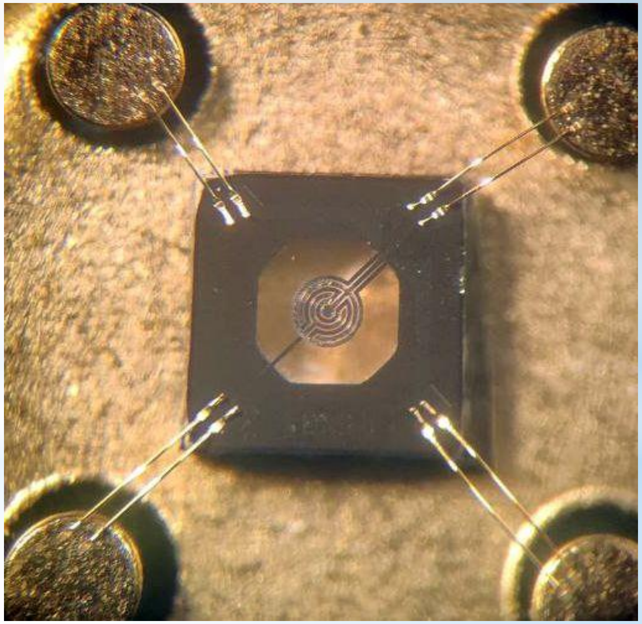
Physical experiment

Gas sensor

Assembly of sensor elements







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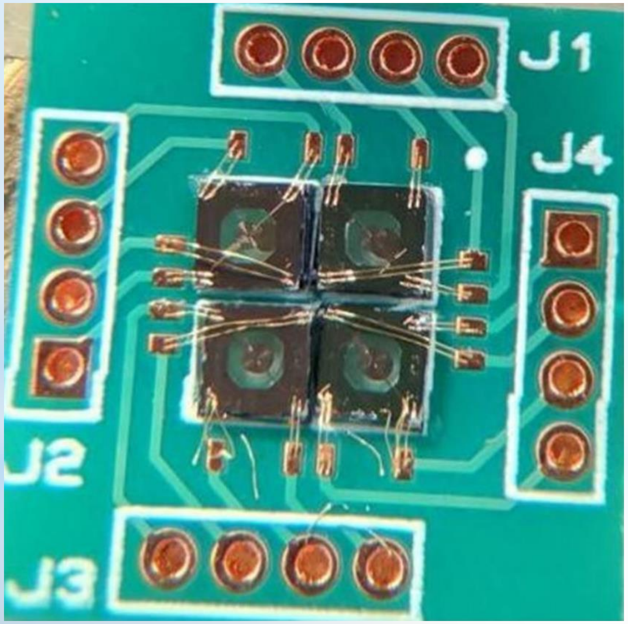


SnO_2

1. SnO_2;
2. SnO_2 – Ru;
3. SnO_2 – Au;
4. SnO_2 – Pt;
5. SnO_2 – Pd;
6. SnO_2 – Cr – Nb;
7. SnO_2 – Si;
8. SnO_2 – Si – Au;

TiO_2

9. TiO_2 – Cr;
10. TiO_2 – Cr – Au;
11. TiO_2 – Nb – Au;
12. TiO_2 – Nb

Binding degree depends on:

- ❑ Type of gas and its concentration
- ❑ Sensor material
- ❑ Temperature

Set of semiconductor sensors with different doping components are used to achieve selectivity when detecting certain gases

Physical experiment

Gas sensor

Heating dynamics

Binding degree depends on:

- ❑ Type of gas and its concentration
- ❑ Sensor material
- ❑ Temperature →

- Binding gas molecules decreasing with temperature increase
- Heating is necessary to bring the sensor to original state
- Cyclic heating and cooling had to be used to ensure the temporal resolution

Physical experiment

Gas sensor

Heating dynamics

Binding degree depends on:

- ❑ Type of gas and its concentration
- ❑ Sensor material
- ❑ Temperature

- The electrical resistance of semiconductor materials also depends on temperature

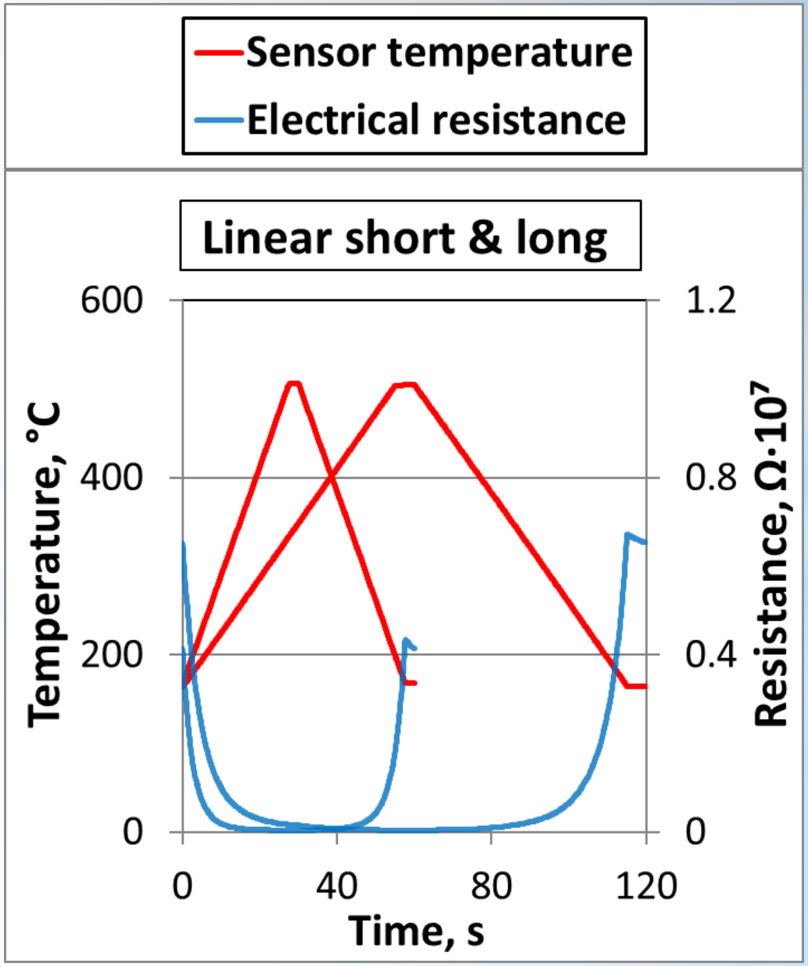
- Binding gas molecules decreasing with temperature increase
- Heating is necessary to bring the sensor to original state
- Cyclic heating and cooling had to be used to ensure the temporal resolution

To increase the selectivity of gas determination, various temperature operating conditions were used: the so-called heating dynamics

Physical experiment

Heating dynamics

- Linear heating and cooling
  - *Linear long*
  - *Linear short*
- Stepwise smooth increase or decrease in temperature
  - *Step up*
  - *Step down*
- Stepwise smooth increase or decrease in temperature and short-term pulsed temperature jumps to maximum
  - *Step up pulse*
  - *Step down pulse*



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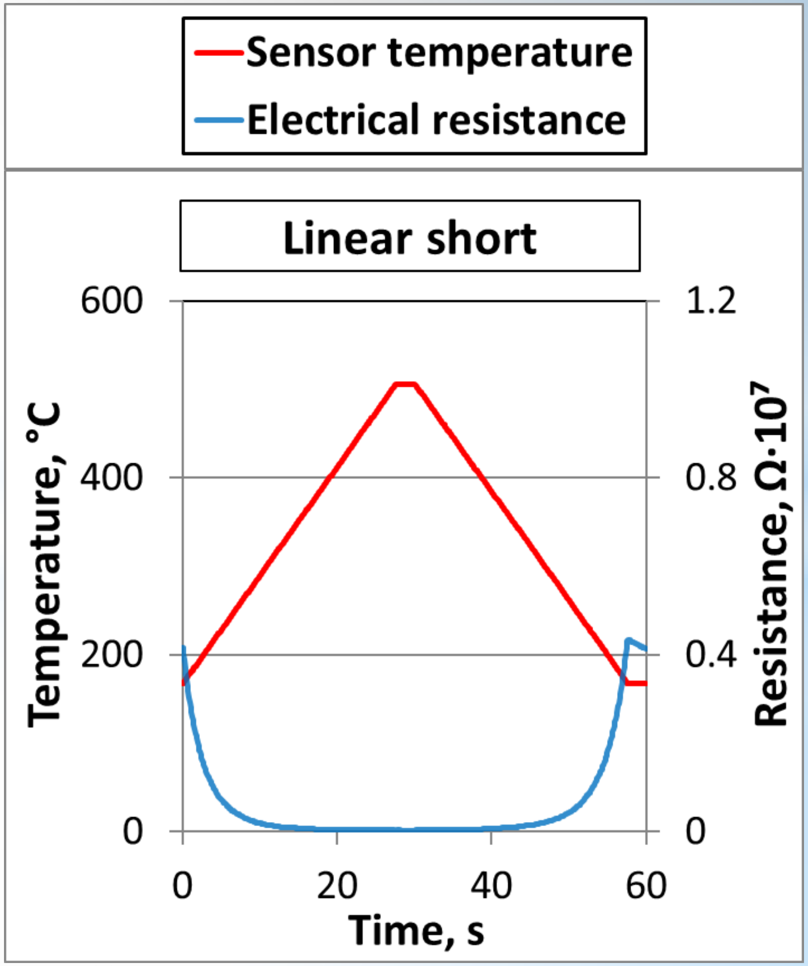

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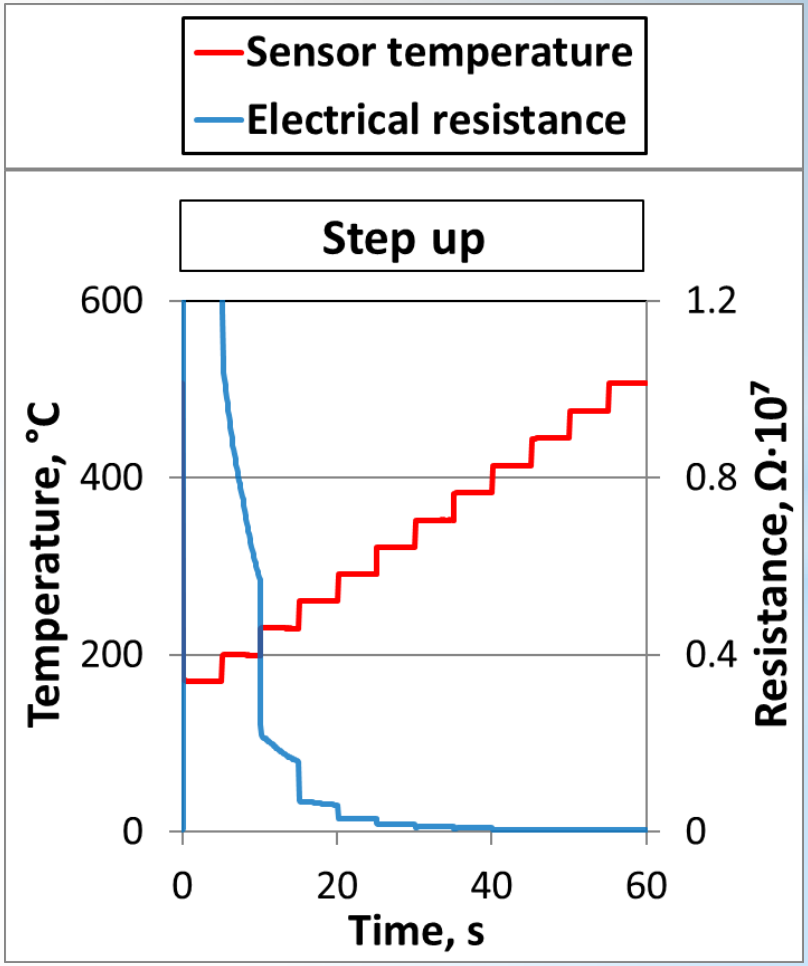

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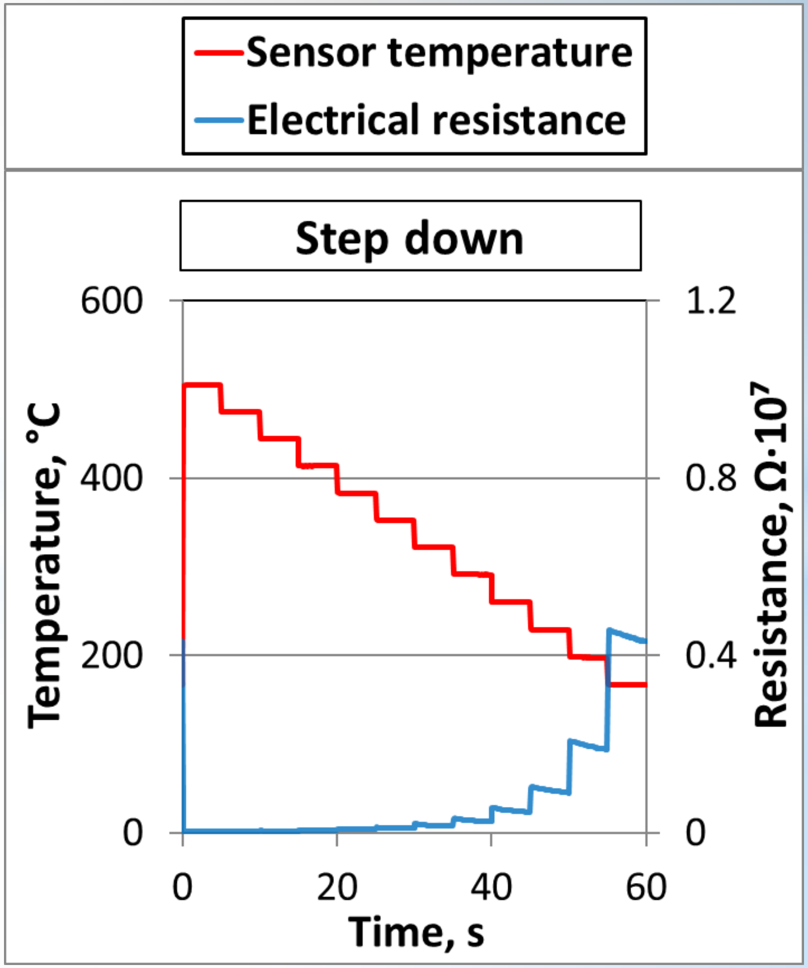

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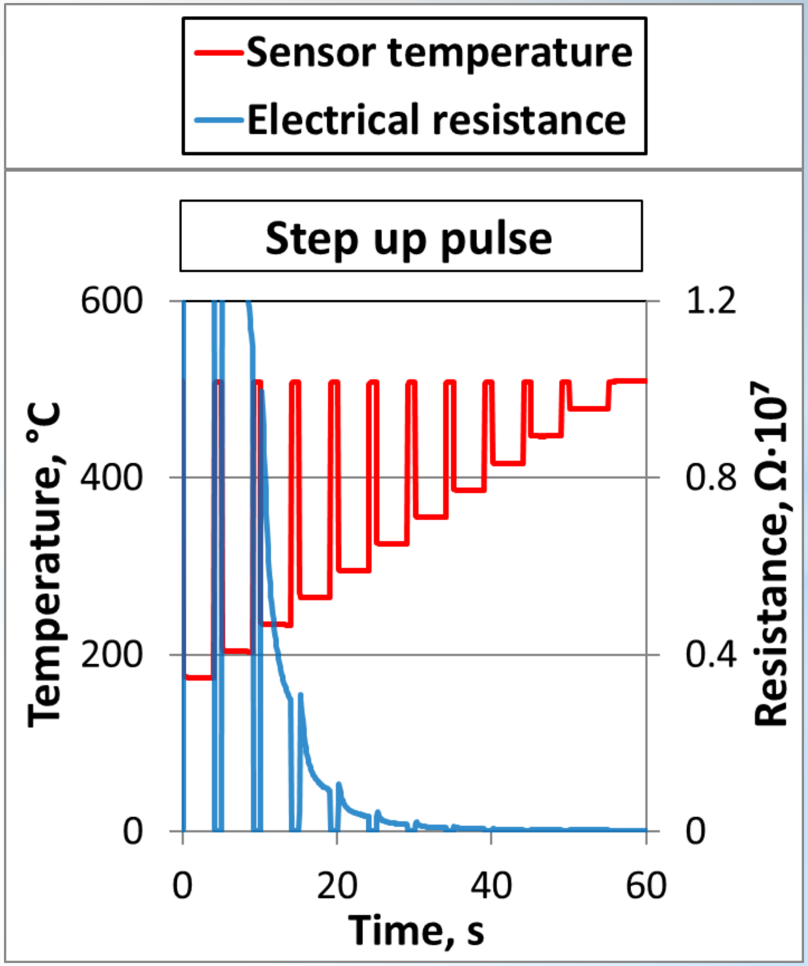

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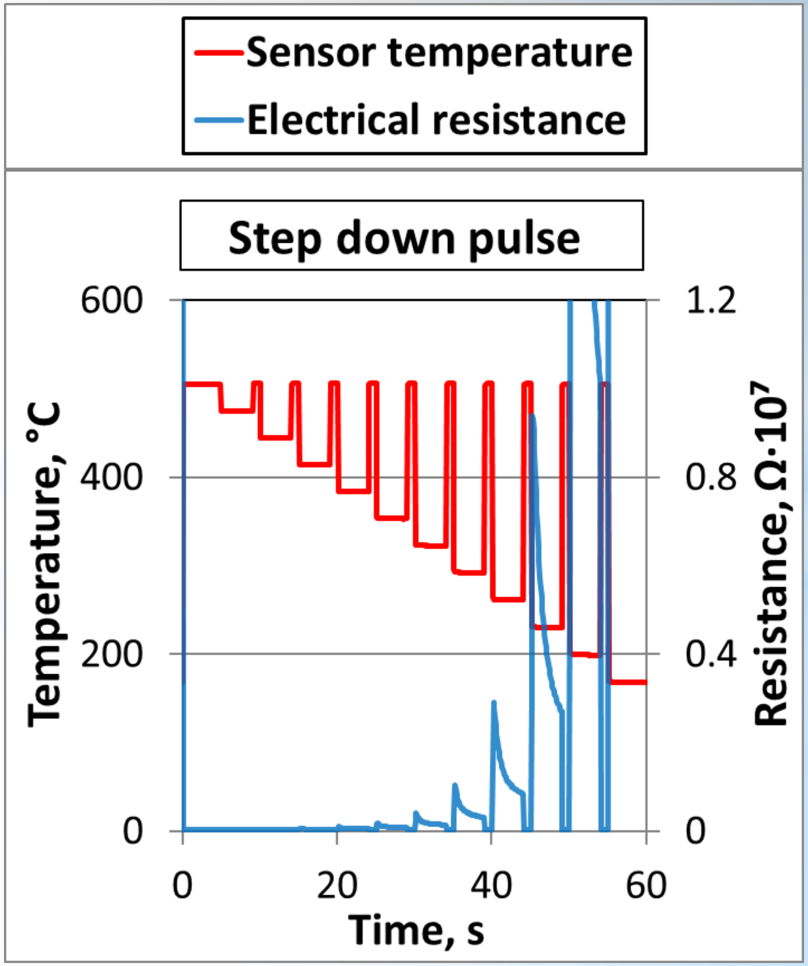
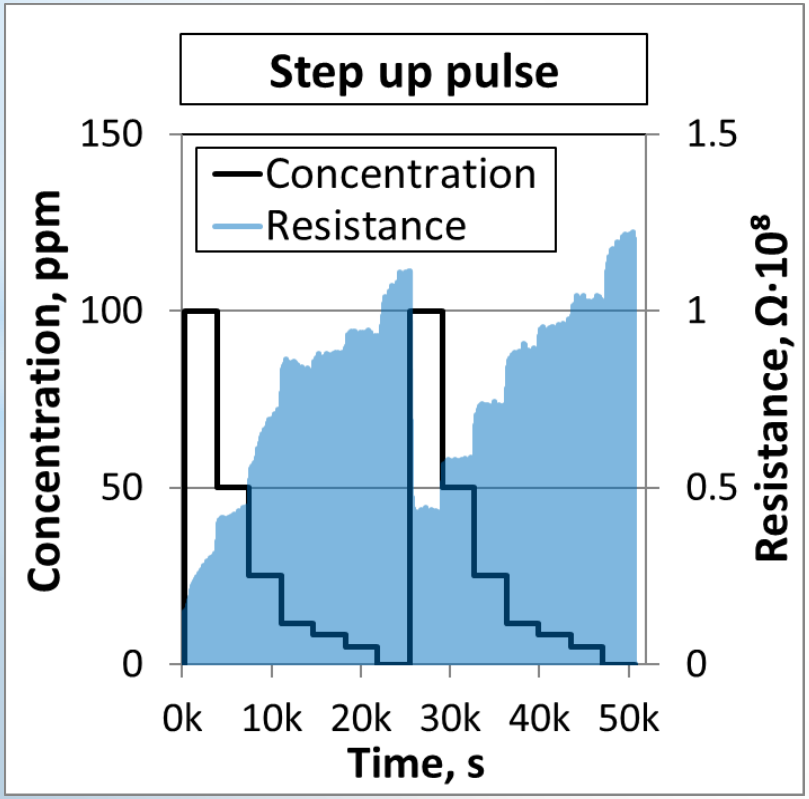
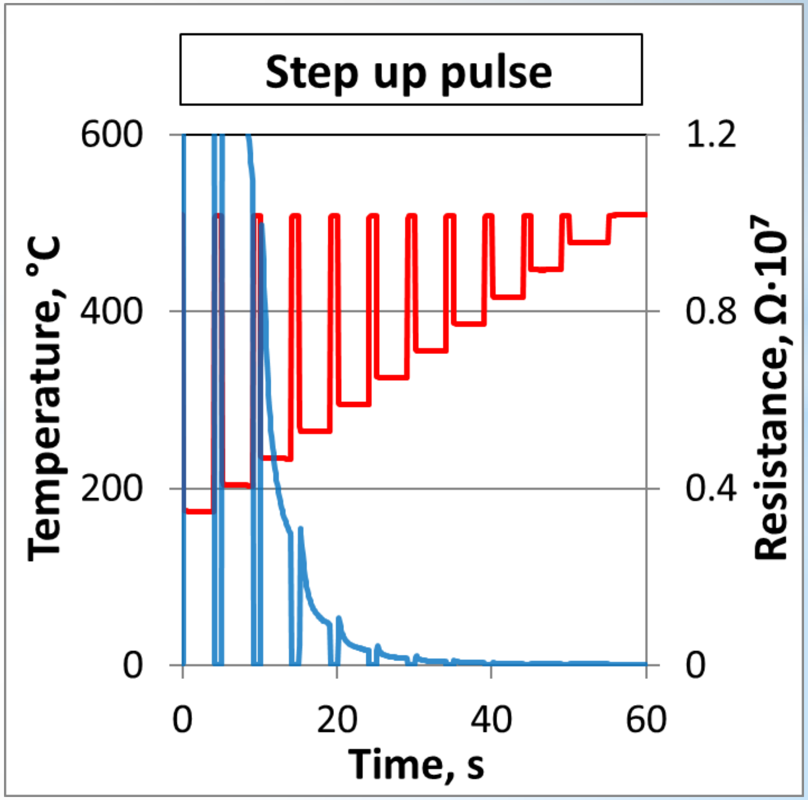


Physical experiment

Gas concentrations

The response forms of the 12 sensors were collected at 6 various heating dynamics in 6 different gas concentrations



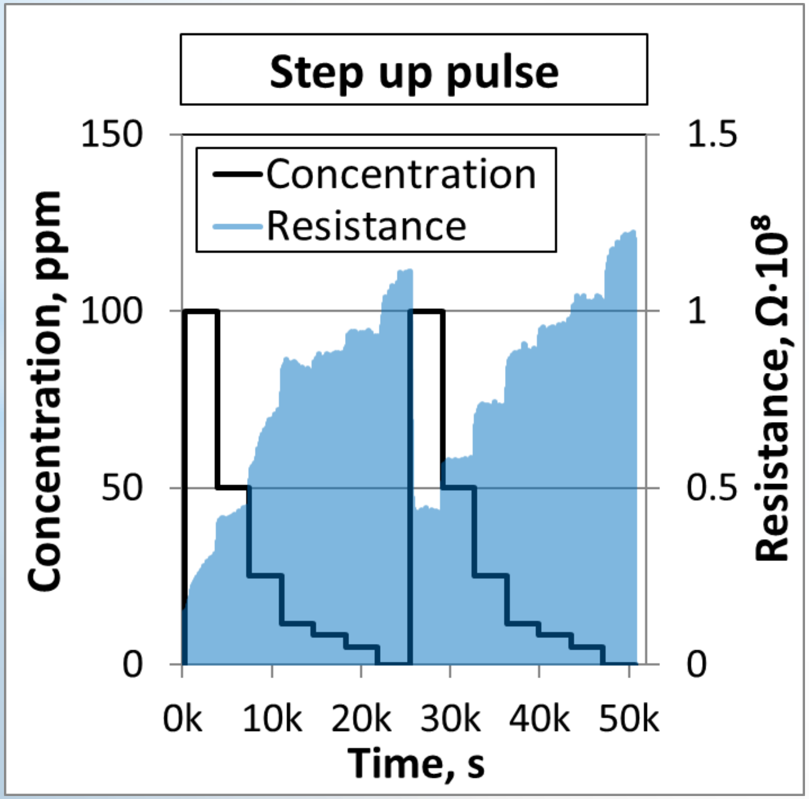


in an atmosphere of clean air, as well as in air with an admixture of gases: CO, H_2, CH_4, NH_3, NO, NO2, H_2S, SO_2, HCOH (only one gas at a time)

Computational experiment

Data Preprocessing

Data preparation and preprocessing steps:



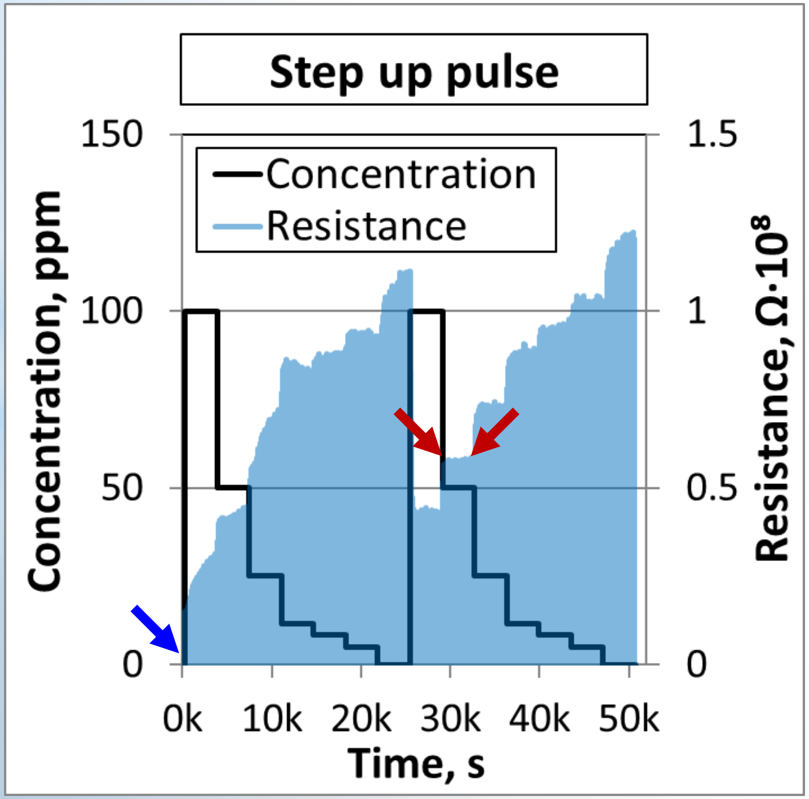
1. Converting data into the format:
   "1 cycle of heating dynamics –
   1 sample of a dataset."

2. Replacing sensor response values
   above 10^9 Ohms
   with a fixed value of 10^9 Ohms,
   and below 10 Ohms
   with a fixed value of 10 Ohms.

Computational experiment

Data Preprocessing

Data preparation and preprocessing steps:



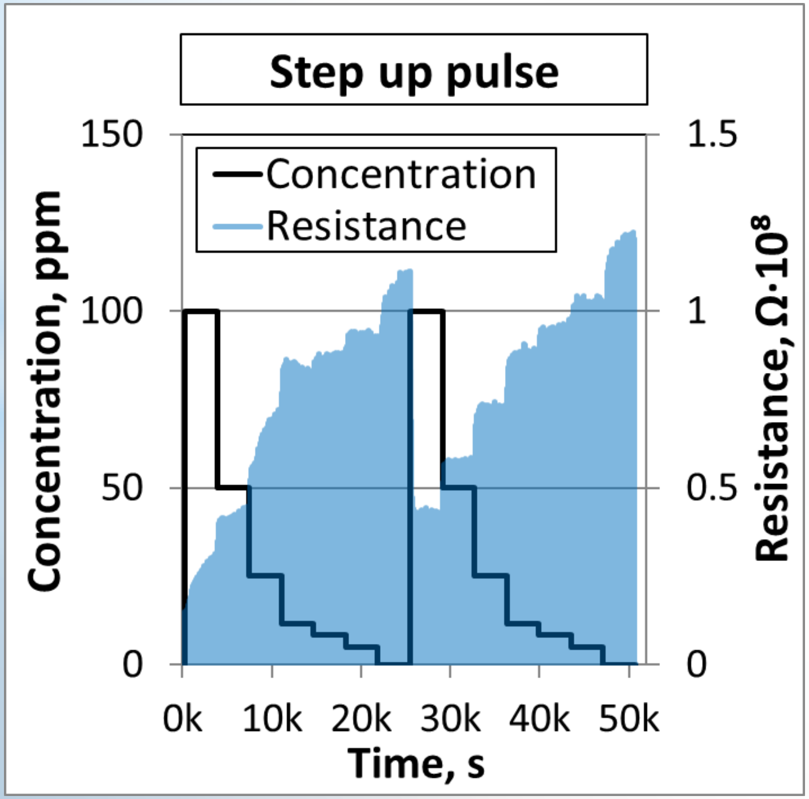
3. Exclusion of data sections where the experimental setup was purged: the first few cycles in each separate experiment.

4. Exclusion of the first few cycles after changing the concentration and several cycles immediately before changing the concentration

Computational experiment

Data Preprocessing

Data preparation and preprocessing steps:



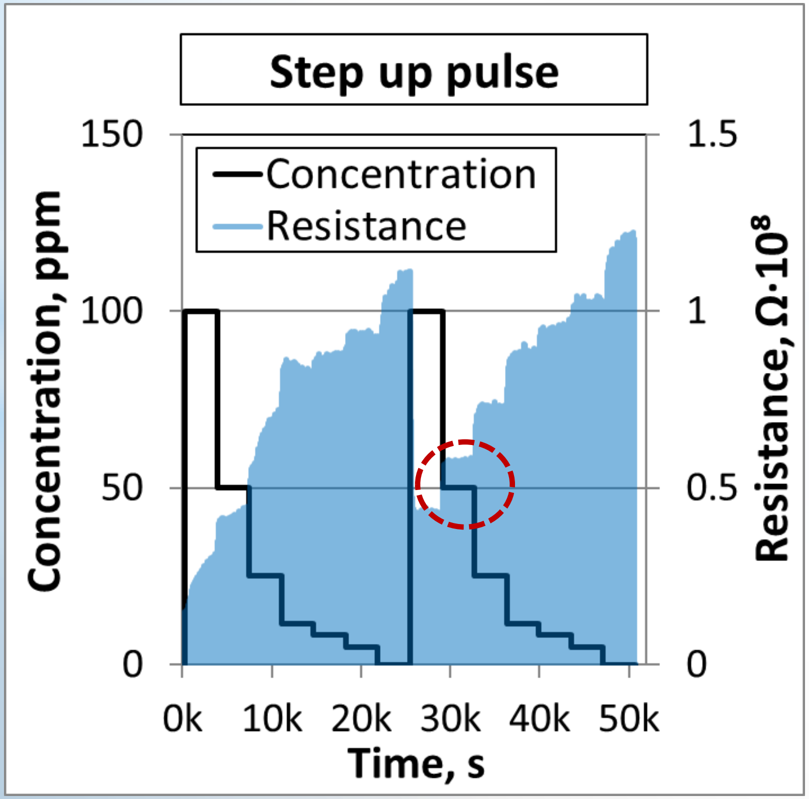
5. Logarithm of sensory response

6. Scaling to minimum and maximum concentration values

Computational experiment

Data Preprocessing

Data preparation and preprocessing steps:



7. Stratified division into subsets.

From each area with a fixed concentration of the gas:

- First ***n*** cycles were selected into training set,
- Next ***m*** cycles – into validation set,
- Subsequent ***k*** cycles – into test set

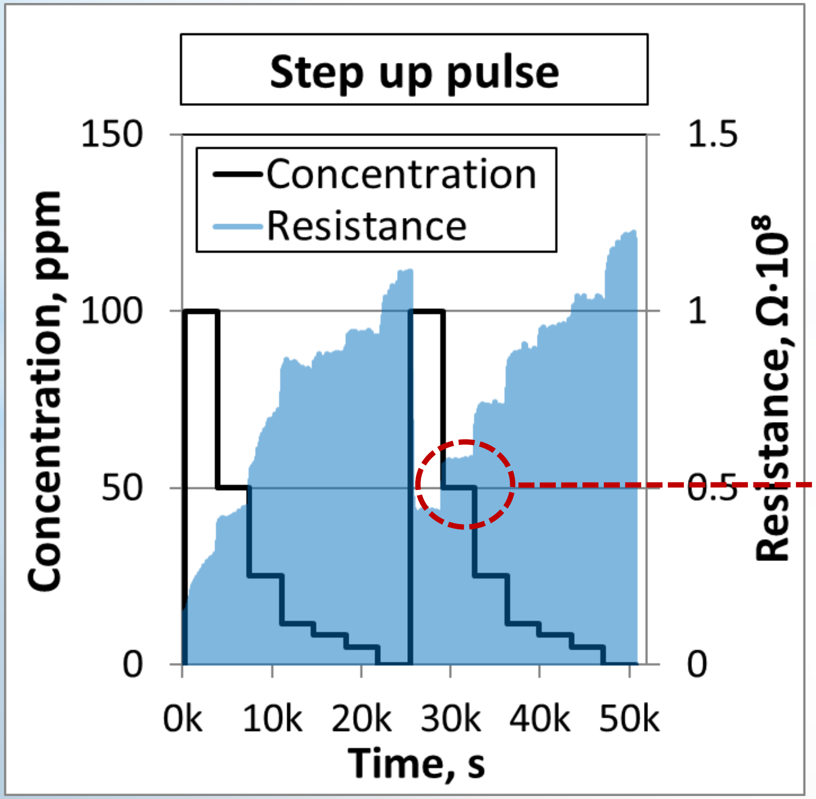
Then the procedure was repeated for other sections with a fixed concentration.

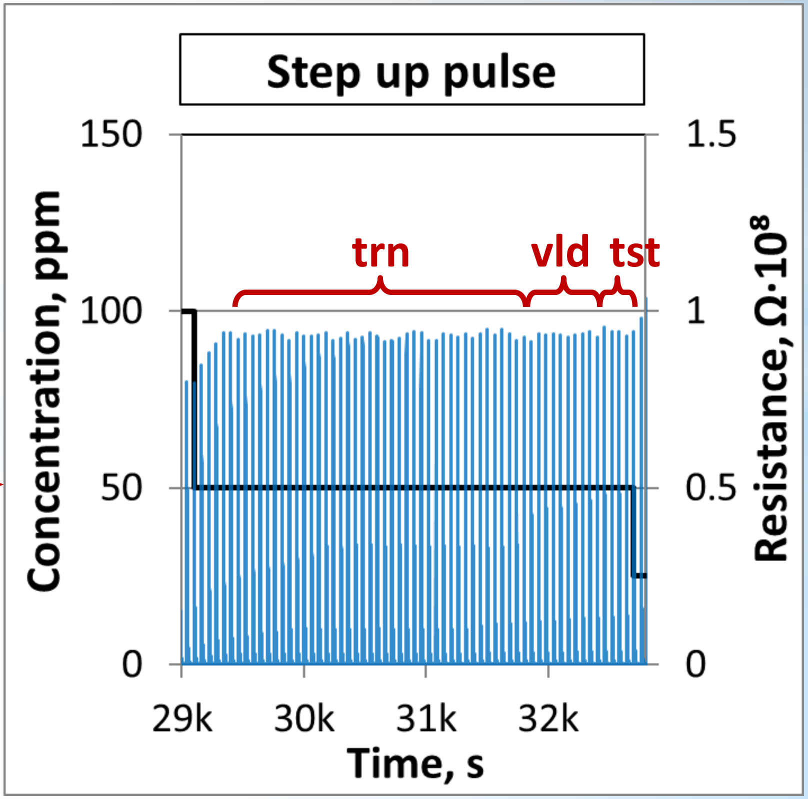
Computational experiment

Data Preprocessing

Data preparation and preprocessing steps:

7. Stratified division into subsets





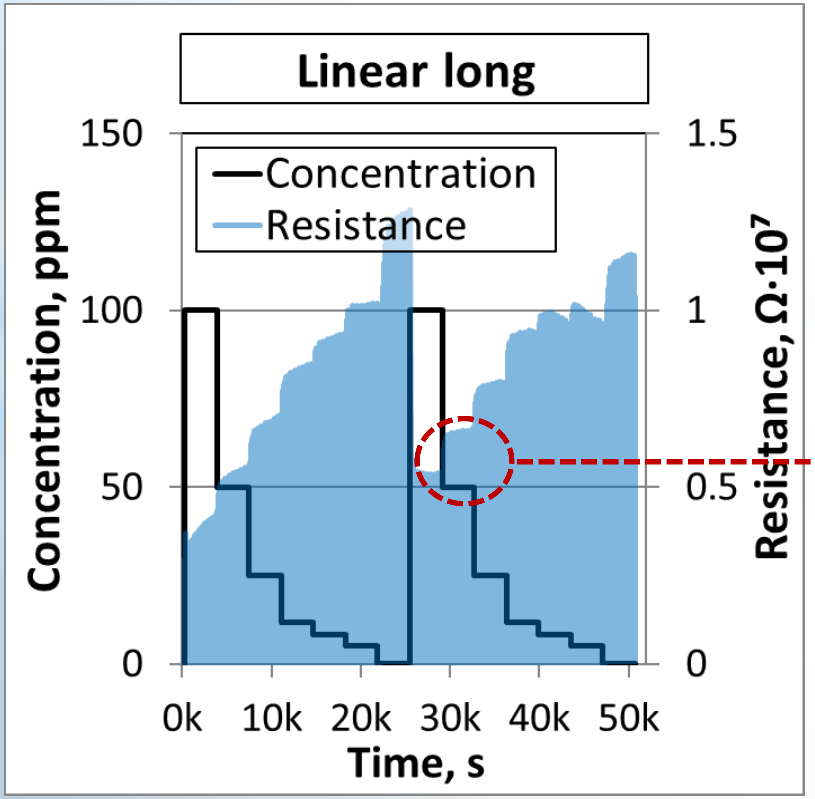
n:***m***:***k*** = *40:10:5*

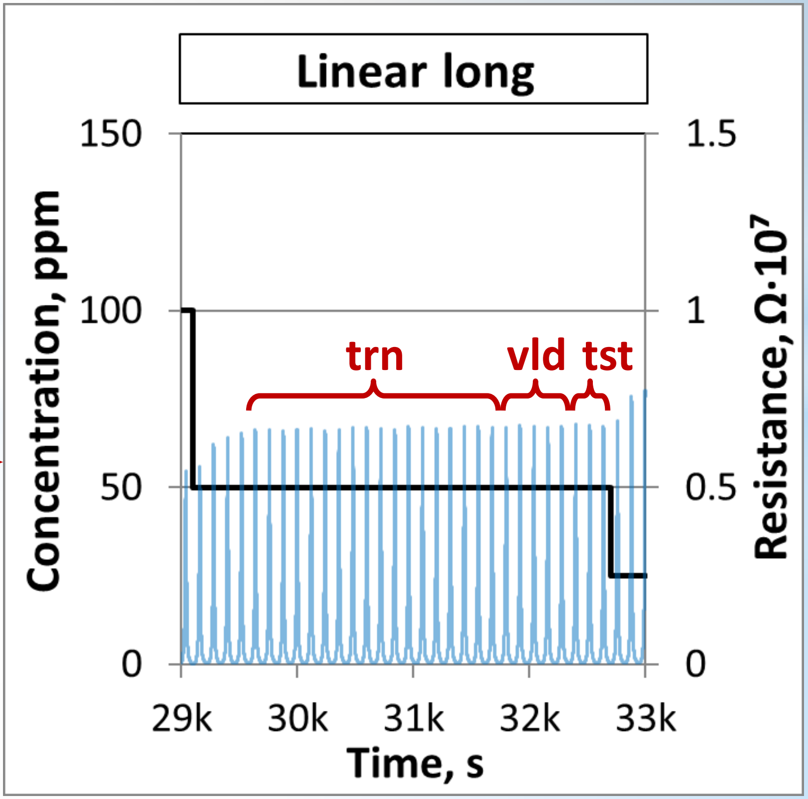
Computational experiment

Data Preprocessing

Data preparation and preprocessing steps:

7. Stratified division into subsets





n:***m***:***k*** = *18:5:3*

Computational experiment

Machine learning methods

- Linear methods
  - Linear regression
  - Lasso
  - Ridge
- Nonlinear methods
  - Multi-layer Perceptron

All methods showed qualitatively similar results

Computational experiment

Results

Quality of the solution (R^2) for Linear regression

Linear long	Sensor No											
gas_name	1	2	3	4	5	6	7	8	9	10	11	12
CH4	1.000	0.998	0.999	0.998	0.996	0.977	0.999	1.000	0.990	0.986	0.992	0.995
CO	0.999	1.000	1.000	1.000	0.999	0.994	0.999	0.999	0.999	0.999	0.999	0.999
H2	1.000	1.000	0.999	0.998	0.998	0.997	0.999	0.998	0.986	0.997	0.994	-17.332
H2S	1.000	1.000	1.000	1.000	1.000	0.993	0.999	0.998	0.999	0.999	0.966	0.961
HCOH	0.999	0.999	0.999	1.000	0.999	0.991	1.000	1.000	1.000	0.999	0.941	0.963
NH3	1.000	0.999	0.999	1.000	0.999	0.986	0.999	1.000	0.999	0.999	0.994	0.974
NO	0.994	0.996	0.993	0.997	0.966	0.972	0.996	0.995	0.986	0.986	0.963	0.821
NO2	0.998	0.999	0.999	0.999	0.990	0.989	0.999	1.000	0.994	0.991	0.891	-2.214
SO2	0.974	0.935	0.948	0.928	0.987	0.803	0.968	0.977	0.930	0.939	0.589	0.882

Linear_short	Sensor No											
gas_name	1	2	3	4	5	6	7	8	9	10	11	12
CH4	0.983	0.973	0.986	0.975	0.984	0.484	0.991	0.976	0.964	0.950	0.888	0.923
CO	0.992	0.991	0.991	0.982	0.991	0.924	0.996	0.995	0.993	0.994	0.923	0.755
H2	0.998	0.998	0.999	0.996	0.994	0.976	0.993	0.996	0.936	0.989	0.873	0.984
H2S	1.000	0.999	1.000	0.999	0.999	0.967	0.999	1.000	0.998	0.998	0.933	0.960
HCOH	0.994	0.995	0.998	0.995	0.993	0.954	0.997	0.998	0.995	0.995	0.926	0.976
NH3	0.997	0.998	0.997	0.996	0.998	0.935	0.997	0.998	0.998	0.999	0.972	0.981
NO	0.964	0.932	0.983	0.983	0.965	0.905	0.983	0.975	0.971	0.959	########	########
NO2	0.176	0.284	0.183	0.485	0.436	-2.300	0.338	0.556	0.476	0.457	0.037	-0.098
SO2	0.824	0.856	0.901	0.920	0.910	0.402	0.795	0.856	0.858	0.805	-0.317	0.164

Computational experiment

Results

Quality of the solution (R^2) for Linear regression

Steps up	Sensor No											
gas_name	1	2	3	4	5	6	7	8	9	10	11	12
CH4	0.998	0.997	0.998	0.996	0.992	0.814	0.998	0.999	0.926	0.880	0.893	0.998
CO	0.998	0.996	0.999	0.996	0.993	0.978	0.998	0.999	0.990	0.991	0.993	0.981
H2	0.998	0.995	0.997	0.993	0.995	0.989	0.998	0.998	0.872	0.953	0.947	0.998
H2S	0.996	0.996	0.999	0.987	0.997	0.974	0.994	0.997	0.970	0.980	0.810	0.630
HCOH	0.995	0.998	0.998	0.995	0.995	0.971	0.998	0.999	0.992	0.993	0.781	0.958
NH3	0.999	0.998	0.997	0.997	0.998	0.953	0.998	0.999	0.996	0.997	0.920	########
NO	0.988	0.990	0.987	0.986	0.977	0.927	0.986	0.976	0.920	0.972	0.862	########
NO2	0.996	0.998	0.995	0.996	0.992	0.982	0.996	0.997	0.895	0.951	0.504	0.889
SO2	0.221	0.821	0.881	0.263	0.954	0.297	-0.712	0.837	0.267	0.180	0.039	0.853

Steps down	Sensor No											
gas_name	1	2	3	4	5	6	7	8	9	10	11	12
CH4	0.903	0.978	-0.222	0.526	0.943	0.620	0.787	0.989	0.877	0.811	0.942	-96.562
CO	0.809	0.871	0.936	0.884	0.585	0.972	0.952	0.962	0.979	0.917	-0.019	-2.905
H2	0.774	0.938	0.997	-0.235	0.726	0.970	-1.094	0.811	0.867	0.869	-19.303	-12.650
H2S	0.998	0.844	0.525	0.855	0.789	0.443	0.918	0.856	0.724	0.864	-0.567	########
HCOH	0.563	0.926	0.576	0.958	0.778	0.956	0.695	0.955	0.880	0.824	0.883	-31.567
NH3	0.987	0.936	-0.171	0.977	0.622	0.522	0.766	0.989	0.943	0.963	0.201	########
NO	-3.018	-1.853	-2.202	0.279	-0.869	0.637	0.936	-2.718	0.868	0.890	########	########
NO2	0.988	0.959	0.976	0.984	0.900	0.836	0.960	0.973	0.705	0.733	0.570	########
SO2	-2.720	-1.849	-4.586	-2.103	0.542	-0.282	-1.780	-2.711	-0.582	-5.860	########	########

Computational experiment

Results

Quality of the solution (R^2) for Linear regression

Steps up pulse	Sensor No											
gas_name	1	2	3	4	5	6	7	8	9	10	11	12
CH4	0.993	0.995	0.997	0.988	0.989	0.834	0.997	0.998	0.939	0.912	0.972	0.991
CO	0.998	0.998	0.999	0.998	0.996	0.991	0.998	0.999	0.989	0.993	0.999	0.990
H2	0.996	0.998	0.981	0.996	0.988	0.947	0.998	0.977	########	0.710	0.893	0.445
H2S	0.999	0.998	1.000	0.997	0.998	0.979	0.997	0.999	0.998	0.999	0.988	0.939
HCOH	0.995	0.996	0.998	0.994	0.996	0.951	0.998	0.999	0.990	0.991	0.966	0.989
NH3	0.996	0.999	0.998	0.998	0.998	0.947	0.998	0.998	0.996	0.997	0.940	0.948
NO	0.991	0.983	0.995	0.981	0.944	0.922	0.992	0.992	0.960	0.960	########	########
NO2	0.987	0.981	0.990	0.992	0.992	0.967	0.982	0.987	0.945	0.934	0.475	0.917
SO2	0.837	0.912	0.880	0.947	0.959	0.051	0.906	0.951	0.636	0.578	0.053	0.232

Steps down pulse	Sensor No											
gas_name	1	2	3	4	5	6	7	8	9	10	11	12
CH4	0.995	0.996	0.996	0.991	0.994	0.797	0.998	0.999	0.938	0.752	0.976	-2.378
CO	0.998	0.998	0.999	0.999	0.994	0.984	0.999	0.999	0.990	0.995	0.998	-37.406
H2	0.999	0.998	0.998	0.996	0.994	0.985	0.997	0.994	0.854	0.972	0.977	########
H2S	0.997	0.999	0.999	0.998	0.999	0.966	0.999	1.000	0.999	0.999	0.981	0.962
HCOH	0.995	0.997	0.997	0.997	0.996	0.970	0.998	0.999	0.991	0.994	0.964	-24.974
NH3	0.998	0.998	0.998	0.998	0.998	0.951	0.999	0.999	0.998	0.997	0.903	0.978
NO	0.990	0.977	0.993	0.989	0.941	0.867	0.972	0.993	0.941	0.963	0.930	########
NO2	0.994	0.992	0.994	0.994	0.992	0.954	0.995	0.996	0.930	0.961	0.896	########
SO2	0.434	0.174	0.537	0.567	0.901	-1.305	0.567	0.733	0.338	-0.422	-0.605	0.332

Computational experiment

Results

Quality of the solution (R^2) for Linear regression

Av. heat dynamic	Sensor No											
gas_name	1	2	3	4	5	6	7	8	9	10	11	12
CH4	0.979	0.990	0.792	0.912	0.983	0.754	0.962	0.993	0.939	0.882	0.944	-15.839
CO	0.966	0.976	0.987	0.976	0.926	0.974	0.990	0.992	0.990	0.982	0.815	-6.097
H2	0.961	0.988	0.995	0.791	0.949	0.977	0.648	0.962	-21.788	0.915	-2.436	-91.065
H2S	0.998	0.973	0.920	0.973	0.964	0.887	0.984	0.975	0.948	0.973	0.685	-48.826
HCOH	0.924	0.985	0.928	0.990	0.960	0.966	0.948	0.992	0.974	0.966	0.910	-8.776
NH3	0.996	0.988	0.803	0.994	0.936	0.882	0.959	0.997	0.988	0.992	0.822	########
NO	0.318	0.504	0.458	0.869	0.654	0.872	0.977	0.369	0.941	0.955	########	########
NO2	0.857	0.869	0.856	0.908	0.884	0.405	0.878	0.918	0.824	0.838	0.562	########
SO2	0.095	0.308	-0.073	0.254	0.875	-0.006	0.124	0.274	0.408	-0.630	-24.963	########

Av. sensors	Heat dynamic					
gas_name	Linear long	Linear short	Steps down	Steps up	Steps down pulse	Steps up pulse
CH4	0.994	0.923	-7.367	0.957	0.671	0.967
CO	0.999	0.961	0.495	0.993	-2.205	0.996
H2	-0.531	0.978	-2.194	0.978	-42.339	-10.443
H2S	0.993	0.988	-24.180	0.944	0.991	0.991
HCOH	0.991	0.985	-1.881	0.973	-1.173	0.989
NH3	0.996	0.989	-29.259	-44.665	0.984	0.984
NO	0.972	###########	###########	###########	###########	###########
NO2	0.720	0.086	###########	0.933	###########	0.929
SO2	0.905	0.664	-78.119	0.408	0.188	0.662

Conclusions

Conclusions

- Best heating dynamics - linear long
  - ✓ Reducing the length (linear short) leads to a deterioration in the quality of the solution
- Heating dynamics with increasing temperature show better results than with decreasing temperature
- Worst sensor - No. 12 (TiO_2 – Nb)
- Applying trained models to repeated measurements taken over time leads to complete breakdown of the solution !!!

Thank you

for your attention!