Supplementary materials

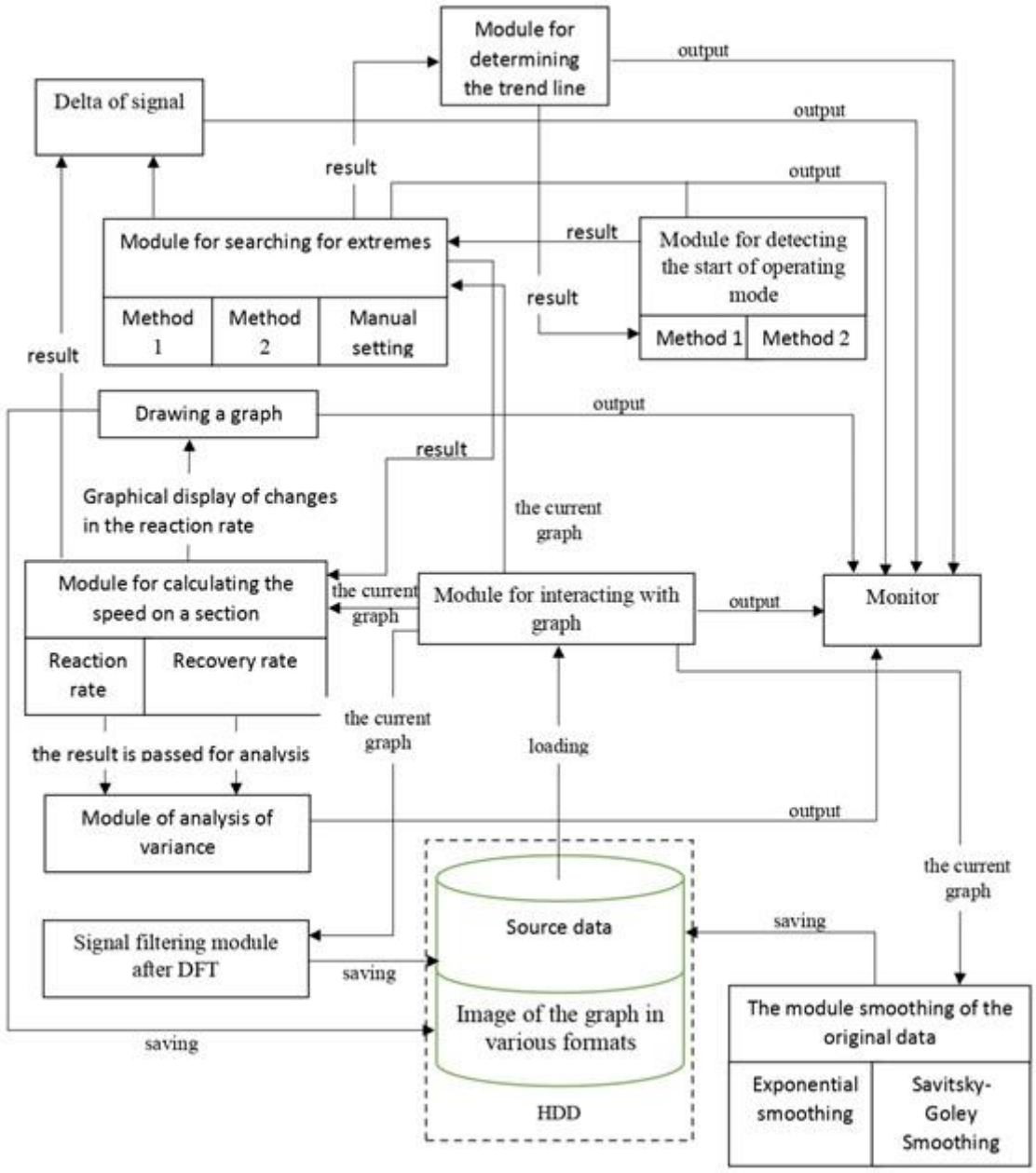

Figure S1. The general signal-processing scheme.

The signal processing circuit includes the main modules (Figure S1):

– Module smoothing of the original data;
– Module for detecting the start of the operating mode;
– Module for searching the extremes;
– Module for calculating the speed on the section;
– Module for determining the trend line.

All incoming data interact with the Module for graphs building and are displayed on the monitor screena.

Signal filtering is carried out using three well-known algorithms in the smoothing Module of the original data:

- exponential smoothing;
- smoothing by the Savitsky-Golay method;

An expert determines the applicability of the algorithm.

Two methods are used to automatically determine the start of the operating mode In the module for determining the start of the operating mode.

In the case of the one method, the algorithm is as follows:

1. The parameters of a straight line in which the measured data approximated are determined in a sliding window. Such an approximation is carried out by the least squares method, which is used to estimate the determination coefficient of this straight line.

2. The determination coefficient is compared with the threshold value. If its value corresponds to the specified threshold, then a decision is made to start the operating mode. When the graph begins to increase sharply, the value of the coefficient of determination begins to decrease sharply and tend to zero. .

3. Displaying the points of the beginning of the operating mode.

4. The window is shifted until the chart limit is reached.

In the case of the second method, the algorithm is as follows:

1. The minimum values of the points between two phases are determined In the sliding window.

2. The window shifts until it is outside the chart values.

3. Displaying the points of the beginning of the operating mode.

The method is chosen depending on the type of graph.

In the module for searching the extremes minimum and maximum are determined. Extremes are divided into:

- global extremes (beginning of the operating mode);
- local extremes.

The Module for calculating the speed in the section implements the building of graphs resistance *vs* time, dividing them into sections: under the gas exposure (reaction rate) and after gas exposure (recovery rate).

Further, the data are sent to the Module of analysis of variance for deeper processing.

At the initial stage, the dependence of the sensor surface resistance on temperature was measured. Figure S2 shows the dependence of the surface resistance taken under various external conditions. Its type represents a typical temperature dependence for a semiconductor. The effect of the airflow on the resistance at a temperature of 80°C becomes insignificant. Thus, this temperature was chosen as the working temperature for further research.

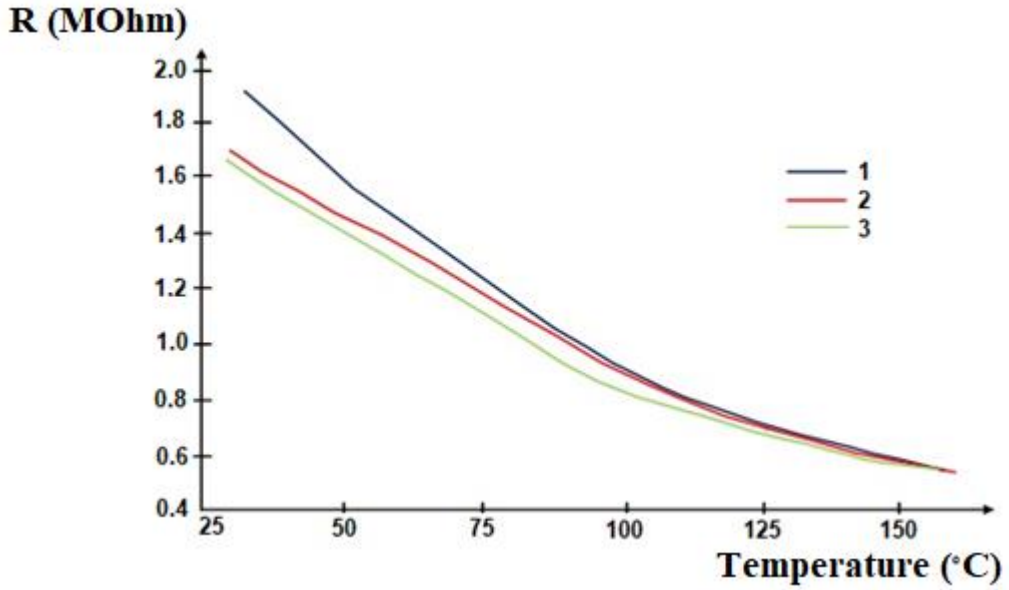

Figure S2. The dependence of the Type 1 sensor resistance on the temperature (1) without exposure; (2) in the airflow; (3) in the nitrogen flow (the flow rate of air and nitrogen 110 ml/min).