Supplementary material

Design of a Decision Support System to Operate a NO_2 Gas Sensor Using Machine Learning, Sensitive Analysis and Conceptual Control Process Modelling

Mohammad Gheibi [1], Hadi Taghavian [2], Reza Moezzi [2,*], Stanislaw Waclawek [2], Jindrich Cyrus [2], Anna Dawiec-Lisniewska [3], Jan Koci [2] and Masoud Khaleghiabbasabadi [2]

[1]Association of Talent under Liberty in Technology (TULTECH), 10615 Tallinn, Estonia
[2]Institute for Nanomaterials, Advanced Technologies and Innovation, Technical University of Liberec, 46117 Liberec, Czech Republic
[3]Department of Advanced Materials Technologies, Faculty of Chemistry, Wroclaw University of Science and Technology, 50-373 Wroclaw, Poland
*Correspondence: reza.moezzi@tul.cz

Table S1. The outcomes of descriptive statistical analysis of response time and sensitivity.

Descriptive statistics	Response time values	Sensitivity values
Mean	325.96	31.24
Standard Error	35.87	8.45
Median	335.00	12.00
Mode	#N/A	12.00
Standard Deviation	179.33	42.24
Sample Variance	32159.21	1784.61
Kurtosis	-1.00	2.28
Skewness	-0.12	1.77
Range	598.00	151.00
Minimum	32.00	1.00
Maximum	630.00	152.00
Sum	8149.00	781.00
Count	25.00	25.00
Largest(1)	630.00	152.00
Smallest(1)	32.00	1.00
Confidence Level(95.0%)	74.02	17.44

Table S2. ANOVA results of the quadratic model for response time answer.

Source	Sum of Squares	df	Mean Square	F Value	p-value (Prob > F)	
Model	759119.2	9	84346.58	99.60824	< 0.0001	significant
A-Fe_3O_4	481.6526	1	481.6526	0.568803	0.4624	
B-NO_2	989.2694	1	989.2694	1.168268	0.2968	
C-Sensitivity	242.378	1	242.378	0.286234	0.6005	
AB	507.8223	1	507.8223	0.599708	0.4507	
AC	67.85406	1	67.85406	0.080132	0.7810	
BC	21.22913	1	21.22913	0.02507	0.8763	
A^2	17.58457	1	17.58457	0.020766	0.8873	
B^2	14084.49	1	14084.49	16.63294	0.0010	
C^2	289.9065	1	289.9065	0.342362	0.5672	

Residual	12701.75	15	846.7831
Cor Total	771821	24	

Table S3. ANOVA results of the cubic model for sensitivity answer.

Source	Sum of Squares	df	Mean Square	F Value	p-value (Prob > F)	
Model	42808.13	19	2253.06	502.2793	< 0.0001	significant
A-Fe_3O_4 additive	17.38261	1	17.38261	3.875142	0.1061	
B-NO_2	22.92347	1	22.92347	5.110378	0.0733	
C-Response Time	27.63673	1	27.63673	6.161114	0.0557	
AB	17.03223	1	17.03223	3.797032	0.1089	
AC	14.87183	1	14.87183	3.315408	0.1283	
BC	16.36063	1	16.36063	3.64731	0.1144	
A^2	11.95904	1	11.95904	2.666054	0.1634	
B^2	12.89767	1	12.89767	2.875304	0.1507	
C^2	8.476267	1	8.476267	1.889632	0.2277	
ABC	19.3308	1	19.3308	4.309456	0.0925	
A^2B	16.32759	1	16.32759	3.639943	0.1147	
A^2C	7.872781	1	7.872781	1.755096	0.2426	
AB^2	22.37084	1	22.37084	4.987178	0.0759	
AC^2	8.230282	1	8.230282	1.834794	0.2336	
B^2C	14.45004	1	14.45004	3.221378	0.1326	
BC^2	13.41669	1	13.41669	2.991011	0.1443	
A^3	5.708059	1	5.708059	1.27251	0.3105	
B^3	11.05561	1	11.05561	2.46465	0.1772	
C^3	9.147208	1	9.147208	2.039206	0.2127	
Residual	22.42835	5	4.485671			
Cor Total	42830.56	24				

Equation S1

Meta.RegressionByDiscretization
Sensitivity % <= 8
| Sensitivity % <= 6
| | NO_2 (mgL^{-1}) <= 2.5: '(570.2-inf)' (3.0/1.0)
| | NO_2 (mgL^{-1}) > 2.5: '(510.4-570.2]' (4.0/1.0)
| Sensitivity % > 6: '(390.8-450.6]' (2.0)
Sensitivity % > 8
| Sensitivity % <= 18
| | Sensitivity % <= 12: '(331-390.8]' (5.0/1.0)
| | Sensitivity % > 12: '(271.2-331]' (3.0)
| Sensitivity % > 18
| | NO_2 (mgL^{-1}) <= 10: '(91.8-151.6]' (3.0/1.0)
| | NO_2 (mgL^{-1}) > 10: '(-inf-91.8]' (5.0/1.0)

Equation S2

M5. Rules
M5 pruned model rules

(using smoothed linear models):
Number of Rules: 3
Rule: 1
IF
Sensitivity % <= 45
Sensitivity % > 9
THEN
Response time (Sec) =
-9.8354 * Sensitivity %
+ 492.5191 [10/10.137%]
Rule: 2
IF
Sensitivity % <= 36.5
THEN
Response time (Sec) =
5.6654 * NO_2 (mgL^{-1})
- 14.7605 * Sensitivity %
+ 542.3807 [9/11.546%]
Rule: 3
Response time (Sec) =
-1.6942 * NO_2 (mgL^{-1})
+ 121.8462 [6/31.184%]

Equation S3

Gaussian Processes
Kernel used:
Linear Kernel: K(x,y) = <x,y>
All values shown based on: Normalize training data
Average Target Value : 0.491571906354515
Inverted Covariance Matrix:
Lowest Value = -0.24231691064261593
Highest Value = 1.0
Inverted Covariance Matrix * Target-value Vector:
Lowest Value = -0.17786731765046457
Highest Value = 0.508428093645485

Equation S4

Meta.RegressionByDiscretization
NO_2 (mgL^{-1}) <= 20
| Response time (Sec) <= 220
| | NO_2 (mgL^{-1}) <= 10: '(61.4-76.5]' (3.0/1.0)
| | NO_2 (mgL^{-1}) > 10: '(76.5-91.6]' (2.0/1.0)
| Response time (Sec) > 220: '(-inf-16.1]' (15.0)
NO_2 (mgL^{-1}) > 20
| Fe_3O_4 additive (%) <= 10: '(16.1-31.2]' (3.0)
| Fe_3O_4 additive (%) > 10: '(121.8-136.9]' (2.0/1.0)

Equation S5

M5. Rules
M5 pruned model rules

(using smoothed linear models) :
Number of Rules : 3

Rule: 1
IF
Response time (Sec) > 165
Response time (Sec) <= 395
THEN
Sensitivity % =
-0.1232 * Response time (Sec)
+ 61.7204 [10/3.664%]
Rule: 2
IF
Response time (Sec) > 265
THEN
Sensitivity % =
-0.1322 * Response time (Sec)
+ 72.5235 [9/4.516%]
Rule: 3
Sensitivity % =
-1.0266 * Response time (Sec)
+ 177.3689 [6/21.572%]

Equation S6
Gaussian Processes
Kernel used:
Linear Kernel: K(x,y) = <x,y>
All values shown based on: Normalize training data
Average Target Value : 0.20026490066225164
Inverted Covariance Matrix:
Lowest Value = -0.18244372703862421
Highest Value = 0.9645847363656818
Inverted Covariance Matrix * Target-value Vector:
Lowest Value = -0.2516629640131336
Highest Value = 0.4036168214263314

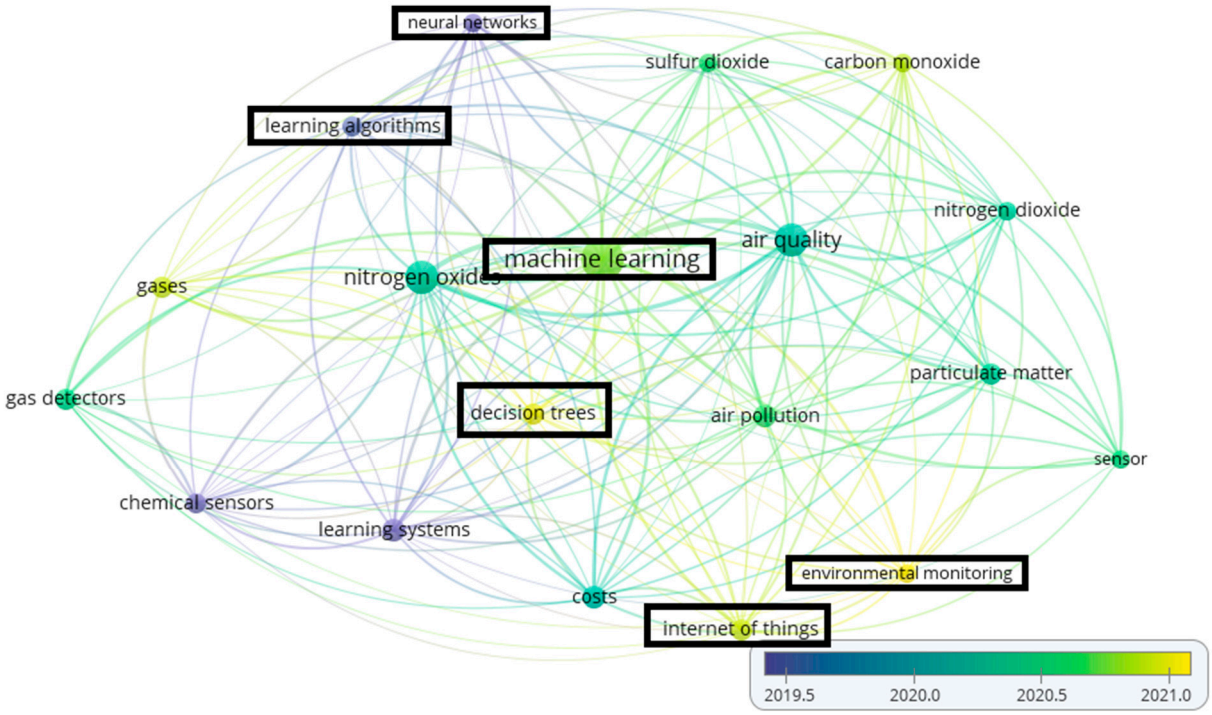

Figure S1. The outputs of the Scientometry analysis of machine learning applications in gas sensor creation based on keyword occurrence.

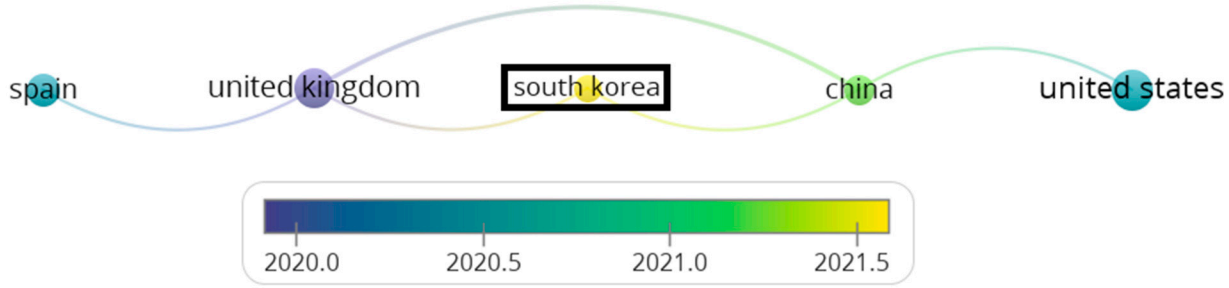

Figure S2. The contribution of countries in the field of artificial intelligence in gas-sensor designing.

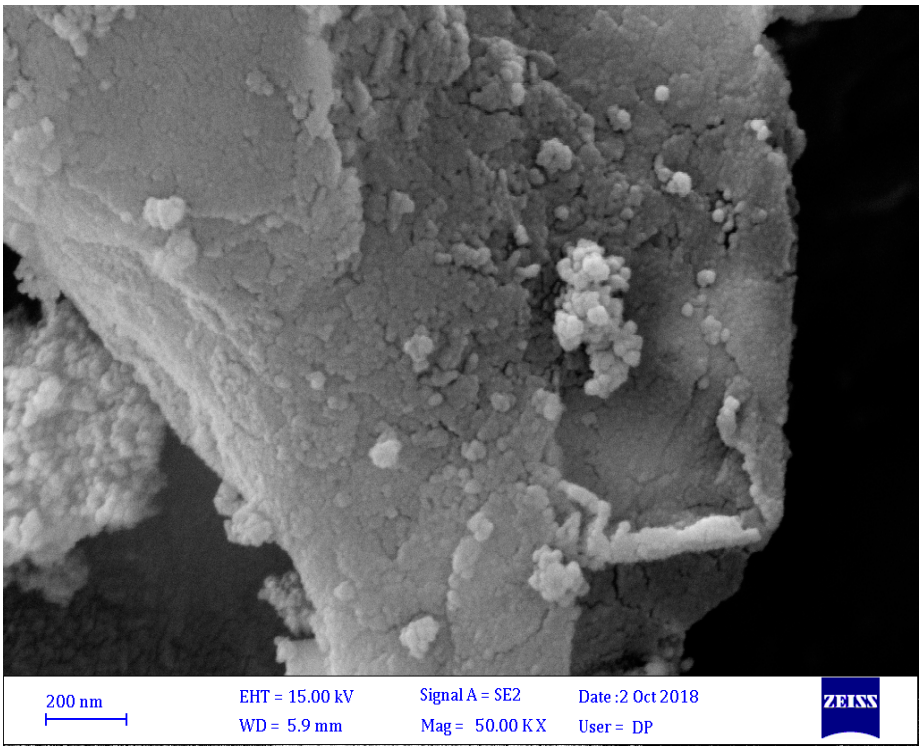

Figure S3. The FESEM characterization of Fe_3O_4-rGOQD-SO_3H as NO_2 gas sensor in this research.