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THE APPLICATION OF NEURAL NETWORKS TO PROPERTY OPTIMIZATION OF POLYMER COMPOSITIONS

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Summary

Preparation of multicomponent, non-flammable polymer-based mixture is time and labour consuming. Many technical attempts have to be carried out in order to obtain the best possible components ratio. That is why artificial neural networks were applied to extend the experimental field of research and to obtain both acceptable mechanical and flame properties of the material. In this paper the results of learning the neural networks as well as their performance at finding the optimum HIPS-based mixture are presented.

Keywords: neural networks, flammability tests, optimization of component ratio

Sztuczne sieci neuronowe w doborze składu mieszaniny polimerowej

Streszczenie

Przygotowanie wieloskładnikowej, trudnopalnej mieszaniny polimerowej o prognozowanych właściwościach mechanicznych jest pracochłonne. Wymaga wykonania wielu prób technologicznych celem uzyskania prawidłowego składu mieszaniny polimerowej wieloskładnikowej z uwzględnieniem kryterium właściwości mechanicznych i palnościowych. Zastosowano zatem sztuczne sieci neuronowe w procesie doboru składników mieszaniny. Przedstawiono proces uczenia się sztucznych sieci neuronowych. Określono również ich wydajność w ustalaniu optymalnego składu mieszaniny na osnowie polistyrenu wysokoudarowego (HIPS).

Słowa kluczowe: sieci neuronowe, badania palności, optymalizacja

1. Data selection and testing the function of the neural networks

In the course of developing a non-flammable polymer composition it was found that there was a contradiction between mechanical and flame properties. Improving the former caused worsening of the latter and inversely. This caused the necessity of using neural networks which would optimize the content ratio in such a way that the material would be both strong and flame resistant [1-3].

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It is known that the potential of neural networks is due to their parallel data processing. They are widely applied in cases where on the one hand it is difficult to find the proper solution, on the other hand – some experimental results are known. The neural networks are treated as "black boxes"; it means that it is of no interest in what way they find the solutions [4-10].

In this paper the neural networks were applied to find the best possible component ratio of the non-flammable HIPS-based mixture. They enabled us to extend the research area so that the desirable properties of the material could be found.

The obtained experimental results of testing the material properties were used for the learning process of the networks. After the process was completed, the networks were used to process the virtual data, that is the one not obtained experimentally.

In this paper the simulation was performed for the following two cases:

- when the mechanical and flame properties were the input data and the component ratio was searched.
- when the component ratio was the input data and the properties were searched.

In the first case the following parameters were introduced:

- as the input data:
  - Oxygen index OI
  - Exposure S
  - Illumination intensity E4
  - Hardness
  - Impact strength
  - Young modulus
  - Tensile strength
- as the results, the percentage ratio of:
  - $Mg(OH)_2$
  - HIPS
  - SBS (Styrene-butadiene-styrene elastomer)
  - SEBS (Styrene-ethylene-butylene-styrene elastomer)

In the second case, based on the percentage ratio of the four components, the properties of the material were searched. In the course of the experimental testing it was found out that impact strength was critical in terms of mechanical properties. The other three mentioned kept at the satisfactory level [11, 12]. That is why it was decided that only impact strength would represent the mechanical properties of the material. Due to the same reason only oxygen index and illumination intensity E4 were selected as the representative parameters of the flame properties. The exposure S kept at a remarkably high level for all the mixtures tested.

2. Selection of the networks type

The learning files were used to determine the most appropriate networks type for solving the given task. It means to find the best possible component ratio in terms of mechanical and flame properties. The networks type was selected according to the procedure used in STATISTICA Neural Networks. In accordance with the theory of neural networks the one of the simplest possible structure should be selected as well as the simplest possible learning algorithm. It results in a short learning time and minimized risk of local minima which, consequently, leads to smaller deviation error. Based on these principles and on the results obtained from testing some types of networks, finely the MLP type and the algorithm of backpropagation were selected. Figures 1 and 2 show the schemes of the networks.

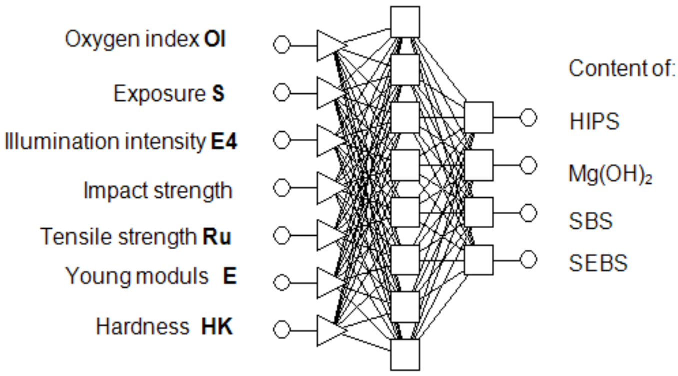

Fig. 1. Scheme of the MLP networks for the first case:
input data – properties, results – component ratio

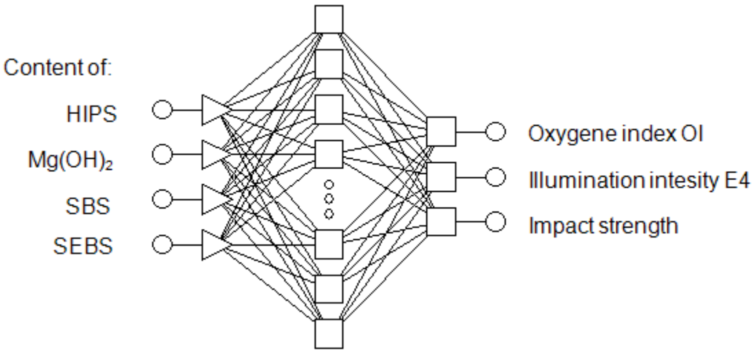

Fig. 2. Scheme of the MLP networks for the second case:
input data – component ratio, results – properties

3. Testing the function of the neural networks based on the experimental data

3.1. Searching the component ratio when the properties are given

In this case, based on the known mechanical and flame properties, the component ratio was to be found. Input and output data are presented at Fig. 1. At Figures 3-5 the plots comparing the experimental and simulated results for the two-component mixture are presented.

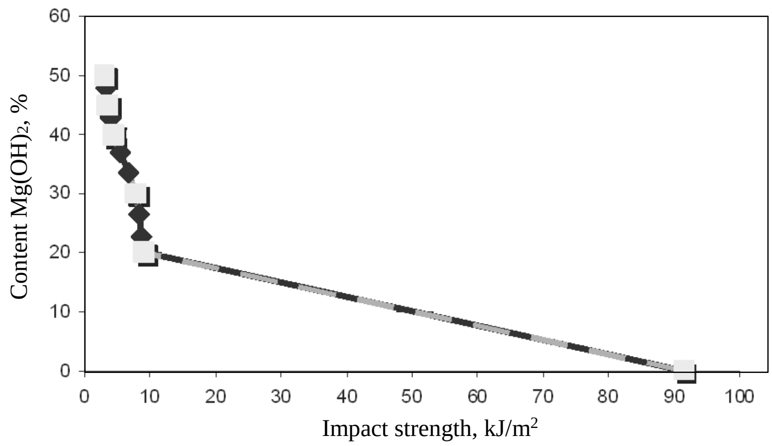

Fig. 3. Plot of $Mg(OH)_2$ content vs. impact strength
(light – experimental results, dark – output data from the networks)

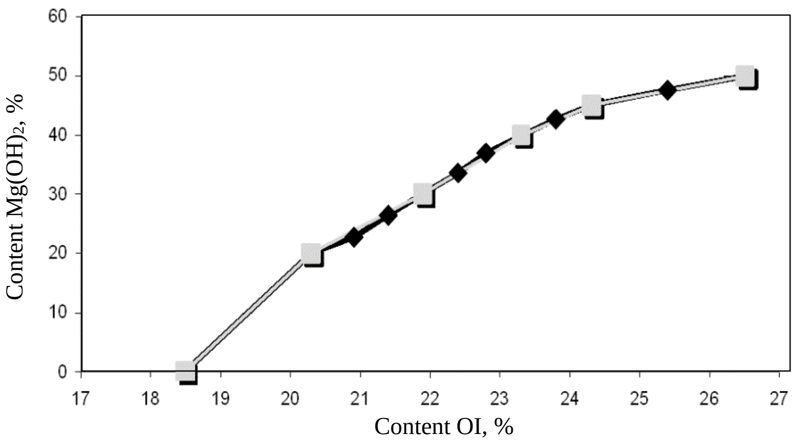

Fig. 4. Plot of $Mg(OH)_2$ content vs. oxygen index OI
(light – experimental results, dark – output data from the networks)

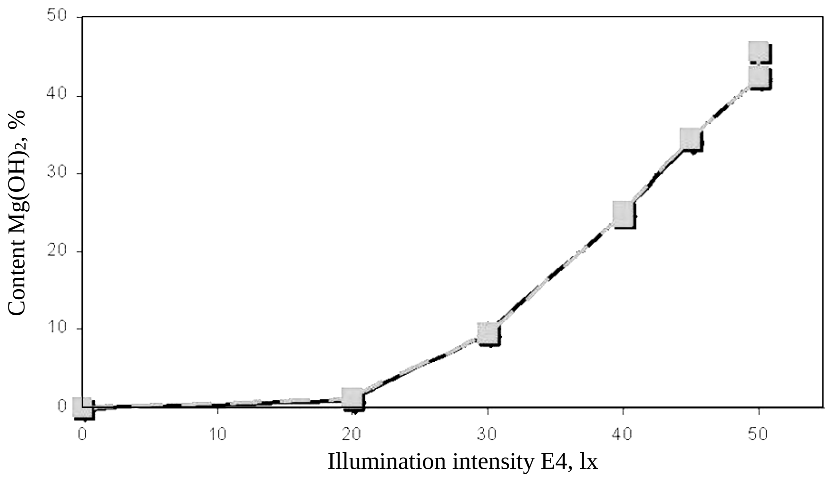

Fig. 5. Plot of $Mg(OH)_2$ content vs. illumination intensity E4 (light – experimental results, dark – output data from the networks; both results almost create a common plot)

The above diagrams show that the experimental results are in good accordance with the output data obtained from the neural networks. It confirms the proper selection of both the network type and the learning algorithm.

In a similar manner the results obtained for three-component system were analyzed. In this case the experimental and simulated sets of mixtures for the same component ratios were compared. At Figures 6, 7, 8 the comparison in the form of bar charts is presented. The numbers denote the following sets of mixtures:

1. experimental results – light:
   HIPS – 35%; $Mg(OH)_2$ – 50%; SBS – 15%
   output data from the networks – dark:
   HIPS- 34,08%; $Mg(OH)_2$ – 50,04%; SBS – 15,08%
2. experimental results – light:
   HIPS – 40,5%; $Mg(OH)_2$ – 55%; SBS – 4,5%
   output data from the networks – dark:
   HIPS – 40,46%; $Mg(OH)_2$ – 54,96%; SBS – 4,48%;
3. experimental results – light:
   HIPS – 55%; $Mg(OH)_2$ – 31,5%; SBS – 13,5%
   output data from the networks – dark:
   HIPS – 31,39%; $Mg(OH)_2$ – 54,98%; SBS – 13,59%;
4. experimental results – light:
   HIPS – 22,5%; $Mg(OH)_2$ – 55%; SBS – 22,5%
   output data from the networks – dark:
   HIPS – 22,41%; $Mg(OH)_2$ – 54,98%; SBS – 22,57%;

It can be seen that for the three-component mixture the networks also performed the simulation satisfactorily; the experimental and simulated values are very close.

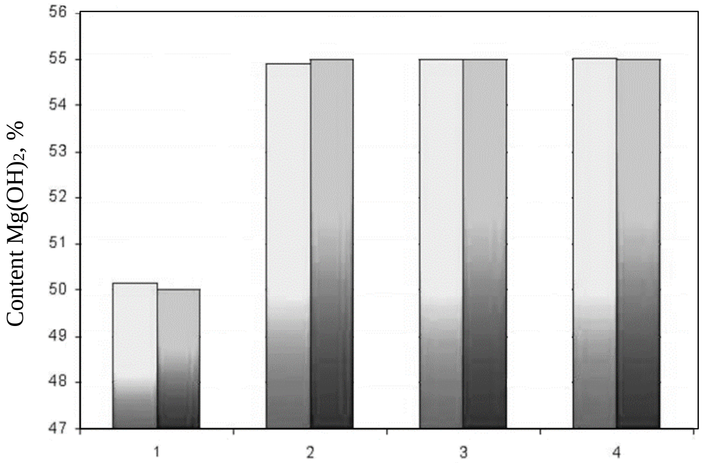

Fig. 6. $Mg(OH)_2$ content for four sets of mixtures,
(experimental results – light output data from the networks – dark)

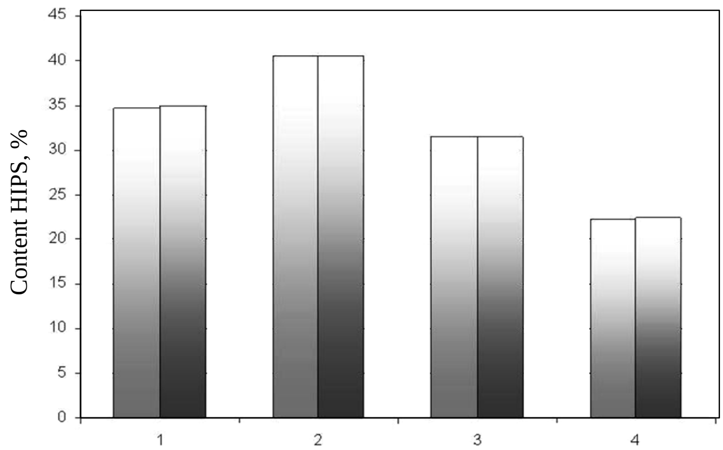

Fig. 7. HIPS content for four sets of mixtures
(experimental results – light, output data from the networks – dark)

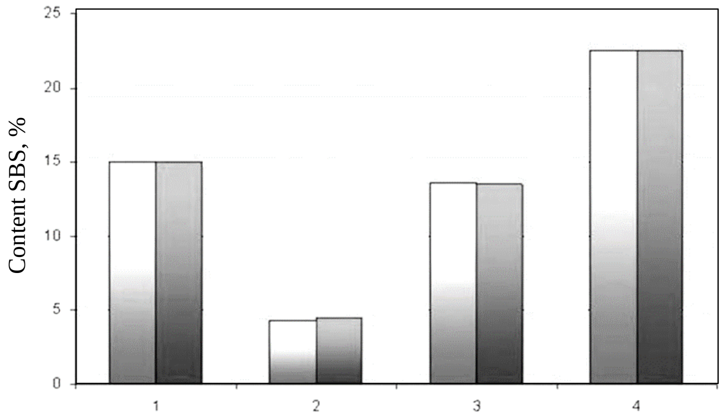

Fig. 8. SBS content for four sets of mixtures
(experimental results – light, output data from the networks – dark)

3.2. Searching the properties of the mixture when the component ratio is given

In the second case the learning file had an inversed structure in relation to the first learning file, that is the component ratio was the input data and the properties of the material were the results. The input and output data are shown at Fig. 2. Figures 9, 10, 11 show the comparison of experimental and simulated results for a two-component mixture.

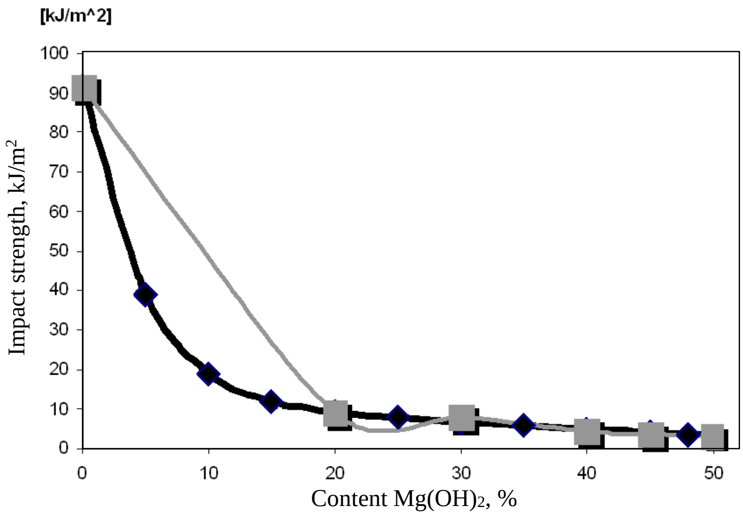

Fig. 9. Plot of impact strength vs. $Mg(OH)_2$ content
(light – experimental results, dark – output data from the networks)

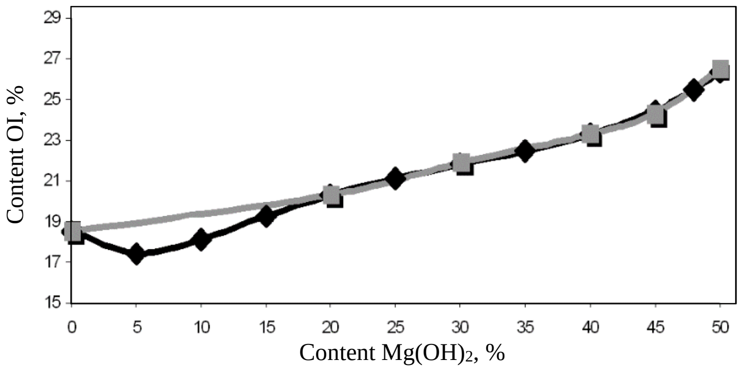

Fig. 10. Plot of oxygen index OI vs. $Mg(OH)_2$ content
(light – experimental results, dark – output data from the networks)

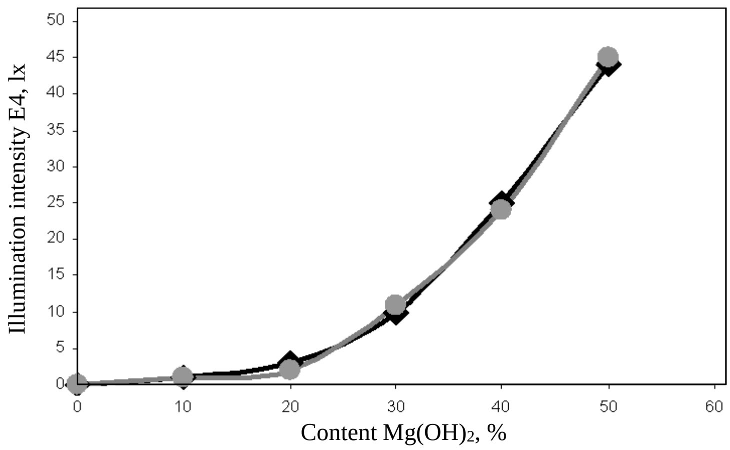

Fig. 11. Plot of illumination intensity E4 vs. $Mg(OH)_2$ content (light – experimental results, dark – output data from the networks both results almost create a common plot)

Summing up the results obtained for the two-component mixture, it is clearly seen that the networks performed correctly; the experimental and simulated values are very close.

As previously, a similar comparison was done for a three-components mixtures. It is illustrated at Figures 12, 13, 14. As can be seen at Fig. 12 only for impact strength some deviations between the experimental and simulated data occur. For the remaining two parameters (Figs. 13 and 14) the convergence is almost perfect.

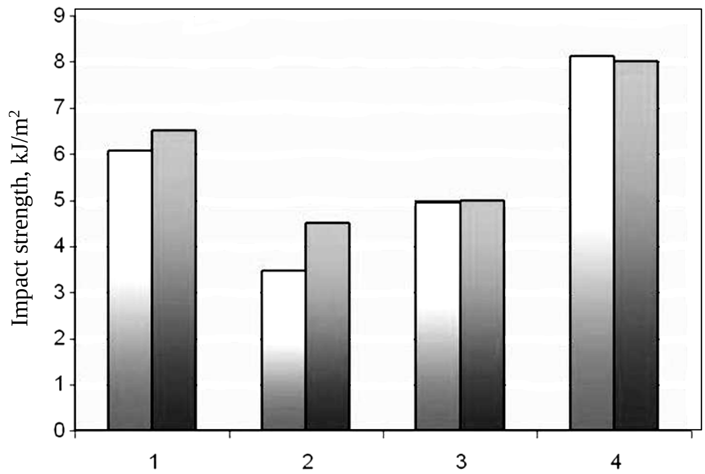

Fig. 12. Impact strength for four sets of mixtures
(experimental results – light, output data from the networks – dark)

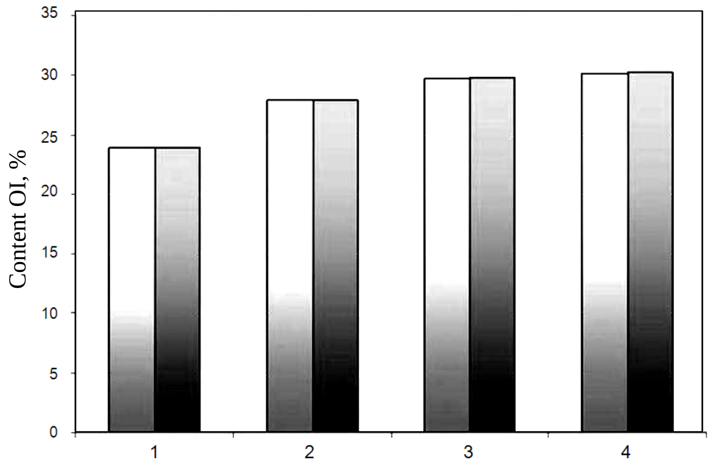

Fig. 13. Oxygen index for four sets of mixtures
(experimental results – light, output data from the networks – dark)

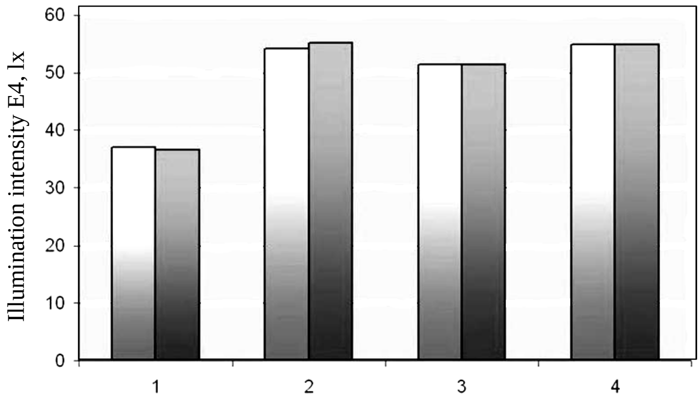

Fig. 14. Illumination intensity for four sets of mixtures
(experimental results – light, output data from the networks – dark)

4. Optimization of the component ratio in terms of the best mechanical and flame properties

4.1. Searching the component ratio based on the desired properties of material

After the learning process had been completed, the proper function of the networks was thoroughly tested. The testing procedure, not described in this paper due to its limited volume, gave positive results which means that the networks performed correctly.

As the next step, the simulation for the virtual (non-experimental) input data was performed. This extended the combination of component ratios above the range obtained from the experiment [11, 12].

Table 1 presents the so called virtual input and output data (results) for the previously mentioned first case (input – properties, output – component ratio). Based on the experimental results the virtual input was selected in such a way that the material should be potentially acceptable in terms of all interesting properties.

As it has already been mentioned, the critical parameters were: oxygen index and impact strength. That is why in table 1 the sets for OI > 28 % and for impact strength close to 5 are printed in bold. These sets, denoted with the numbers 40 to 45, fulfill the requirements. At the bar chart (Fig. 15) the bars related to those sets are framed in bold. For the marked sets the obtained “virtual material” is both non-flammable and mechanically acceptable even though the impact strength is not very high.

Table 1. Simulation for the first case (input – properties, output – component ratio)

No.	Input							Output		
	OI, %	**S, lxs**	**E4, lx**	**HK, MPa**	**Impact strength, kJ/m^2**	**Young Moduls, MPa**	**Ru, MPa**	**$Mg(OH)_2$, %**	**HIPS, %**	**SBS, %**
	1	2	3	4	5	6	7	8	9	10
7	20,9	7941	3,9	48,8	8,72	3623	18	24,74	75,85	0,64
8	21,4	8674	6,63	70,2	8,29	4179	17,4	27,61	72,79	0,44
12	22,4	10448	14,6	94,9	6,71	4605	17,4	33,48	66,17	0,32
13	22,8	11469	19,7	97,8	5,51	4751	17,1	36,83	62,74	0,39
17	23,8	13070	29,6	105,8	3,94	5742	16,4	42,70	56,60	0,61
21	25,4	15075	38,4	116,4	3,275	6931	15,5	47,58	52,34	0,071
28	24,4	16122	38,5	71,9	6,32	5386	15,6	50,96	34,80	14,16
29	24,8	16353	40,3	73,8	6,12	5244	15,5	51,88	34,80	13,17
30	25,2	16584	42,1	75,7	5,92	5102	15,4	52,71	34,94	12,17
31	25,6	16815	43,9	77,6	5,72	4960	15,3	53,42	35,21	11,14
32	25,9	17046	45,7	79,5	5,52	4818	15,2	54,02	35,44	10,27
33	26,3	17277	47,5	81,4	5,32	4676	15,1	54,48	36,08	9,16
34	26,6	17508	49,3	83,3	5,12	4534	15	54,79	36,77	8,13
35	27	17739	51,1	85,2	4,92	4392	14,9	54,97	37,80	6,93
36	27,4	17970	52,9	87,1	4,72	4250	14,8	55,00	39,01	5,73
40	**28,3**	**18173**	**54,6**	**87,5**	**4,59**	**4086**	**15,8**	**54,98**	**39,93**	**5,24**
41	**28,6**	**18123**	**54,1**	**86,1**	**4,66**	**4059**	**15,9**	**55,00**	**39,02**	**6,18**
42	**28,9**	**18073**	**53,5**	**84,7**	**4,73**	**4032**	**16**	**55,03**	**37,63**	**7,53**
43	**29,1**	**18023**	**52,9**	**83,3**	**4,79**	**4006**	**16,1**	**55,00**	**36,37**	**8,80**
44	**29,3**	**17973**	**52,3**	**81,9**	**4,86**	**3979**	**16,2**	**54,99**	**34,81**	**10,33**
45	**29,5**	**17923**	**51,8**	**80,5**	**4,92**	**3953**	**16,4**	**54,99**	**33,24**	**11,85**

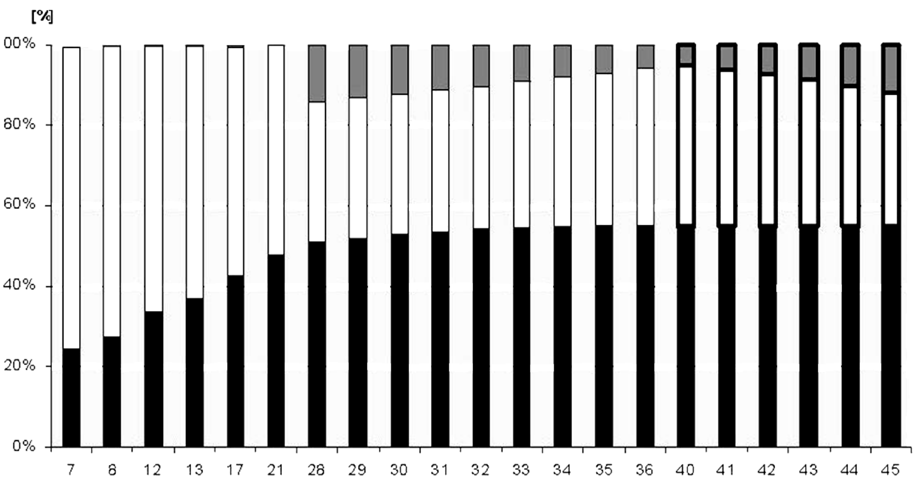

Fig. 15. Component ratio for the virtual, non-flammable mixture obtained as the result of simulation for the first learning set (input – properties, output – component ratio). Black – $Mg(OH)_2$ content, white – HIPS content, grey – SBS content. Framing – optimum sets

4.2. Searching properties of the material based on the component ratio

In this case, the experiment was repeated, yet in the inversed direction. As the input data served the component ratio while the properties of the material were the result of the simulation which is presented in Table 2 and at Figs. 16, 17, 18. As previously, the best results are printed in bold in Table 2.

Table 2. Simulation for the second case (input – component ratio, output – properties)

No.	**Input**			**Output**		
	$Mg(OH)_2$, %	**HIPS, %**	**SBS, %**	**Impact strength, kJ/m^2**	**OI, %**	**E4, lx**
	1	2	3	5	6	7
7	24,74	75,85	0,64	11,95	19,27	0,02
8	27,61	72,79	0,44	18,89	18,12	0,05
12	33,48	66,17	0,32	7,80	21,12	4,66
13	36,83	62,74	0,39	38,99	17,43	1,87
17	42,70	56,60	0,61	5,76	22,47	16,69
21	47,58	52,34	0,07	3,49	25,48	39,10
28	50,96	34,80	14,16	6,51	26,21	40,81
29	**51,88**	**34,80**	**13,17**	**7,46**	**29,09**	**47,08**
30	**52,71**	**34,94**	**12,17**	**7,42**	**29,83**	**50,90**
31	**53,42**	**35,21**	**11,14**	**7,85**	**30,03**	**52,97**
32	54,02	35,44	10,27	6,53	27,98	44,57
33	**54,48**	**36,08**	**9,16**	**6,94**	**28,75**	**46,37**
34	**54,79**	**36,77**	**8,13**	**7,12**	**29,41**	**48,72**
35	**54,97**	**37,80**	**6,93**	**6,15**	**28,20**	**45,54**
36	55,00	39,01	5,73	3,59	27,87	53,60
40	54,98	39,93	5,24	4,43	28,40	50,81
41	55,00	39,02	6,18	4,85	29,53	51,25
42	**55,03**	**37,63**	**7,53**	**5,77**	**30,59**	**52,65**
43	55,00	36,37	8,80	4,00	26,66	48,99
44	54,99	34,81	10,33	4,38	25,64	45,07
45	54,99	33,24	11,85	4,72	24,79	41,76

At Figure 16 it can be seen that impact strength is highest for sets 7, 8 and 13. It is related to the highest HIPS content and to the lowest $Mg(OH)_2$ content (see table 2) which, in turn, decreases the flame and smoke parameters (high smoke emission, low oxygen index – see Figs. 17, 18). As the material is rejected for OI < 28%, sets 7, 8 and 13, in spite of high impact strength could not be taken into account.

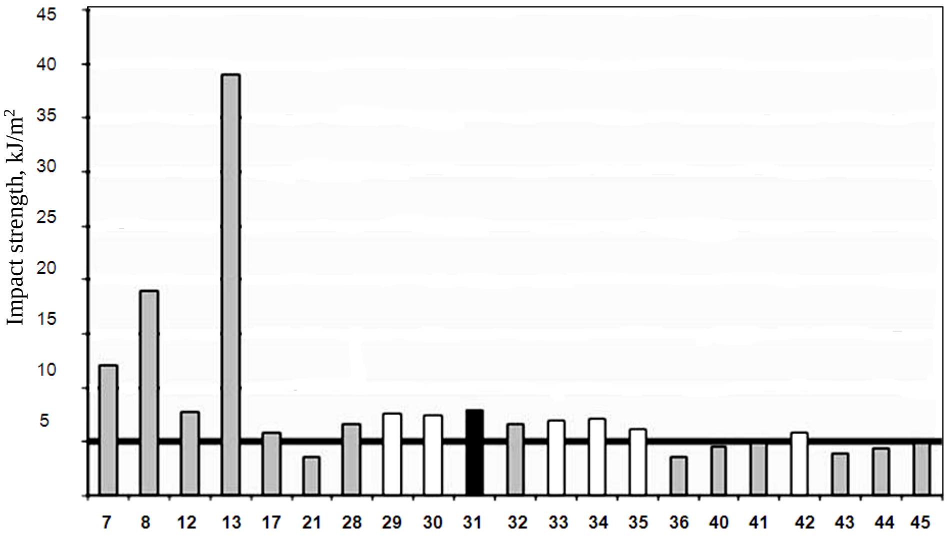

Fig. 16. Impact strength for the sets of virtual material obtained as the result of simulation

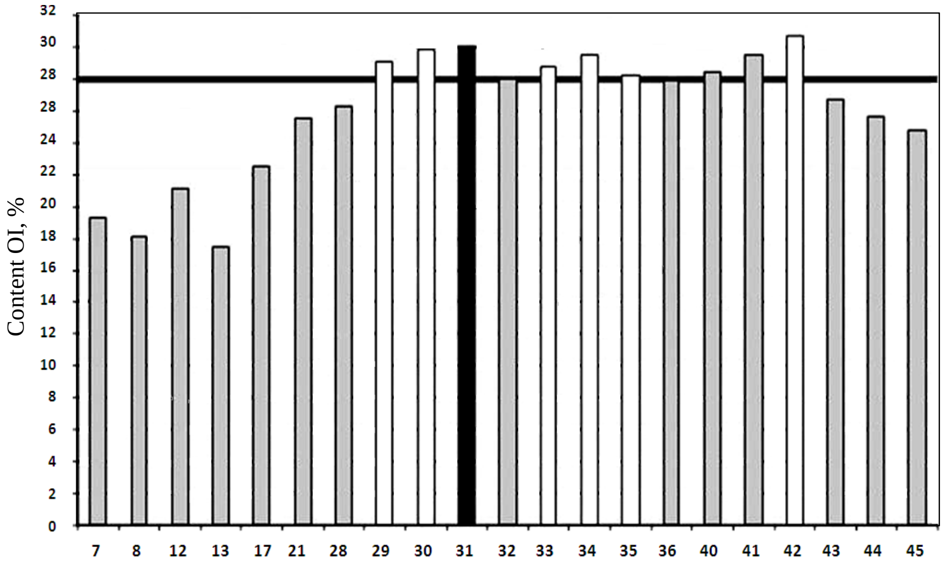

Fig. 17. Oxygen index for the sets of virtual material obtained as the result of simulation

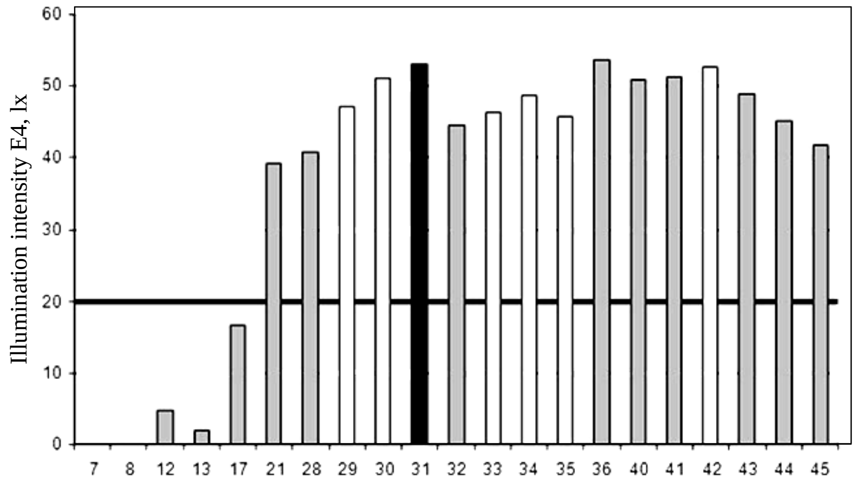

Fig. 18. Illumination intensity for the sets of virtual material obtained as the result of simulation

It is known that oxygen index is mostly effected by the $Mg(OH)_2$ content which unfortunately decreases impact stress remarkably. That is why, when optimizing the properties of the material, this compound should be introduced in a smallest possible amount which keeps the oxygen index above 28%. This occurs for the sets 29-31; 33-35; 42 which is seen at Fig. 17 (white bars).

The next parameter, important because of the smoke emission is the illumination intensity E4. The requirement is that its value should be above 20 lx; below this limit materials are regarded as dangerous because of high smoke emission. In the case of the interesting sets marked in white it makes no problem because E4 keeps over 40 lx (Fig. 10). As it is for OI, the E4 is also mostly effected by $Mg(OH)_2$ content.

The simple procedure of selecting the best possible component ratio in terms of impact strength, oxygen index and illumination intensity is presented in Fig. 19. Following the procedure it could be found that among the acceptable sets (white bars in Figs. 4, 5, 6) the best was the one denoted with number 31 (black bar).

It fulfills all requirements demanded for a non-flammable, mechanically strong material. The oxygen index is above the limit of 28%, illumination intensity E4 is much above the required minimum of 20 lx, impact strength is the highest of all the sets thus meeting the flame and smoke requirements.

It is worthwhile to notice that set 31 is very similar to sets obtained as the result of the simulation in the reverse direction. These are the sets 40-45 of the following component contents:

- 55% $Mg(OH)_2$
- 40-33% HIPS
- 5.25-11.6% SBS

while set 31 contents:

- 53.4% $Mg(OH)_2$
- 35.22% HIPS
- 11.4% SBS.

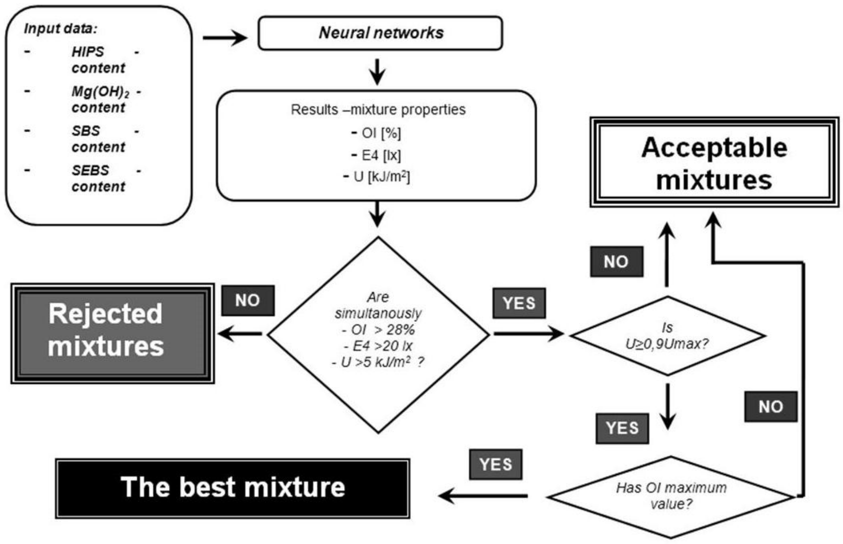

Fig. 19. The algorithm of selecting the best possible component ratio

It can be concluded that the optimum component ratio has been found which on one hand is of practical importance, on the other hand confirms the applicability of neural networks for solving this kind of tasks.

5. Conclusions

- The simulation performed by the networks allowed for finding the optimum component ratio of the non-flammable, HIPS-based mixture.
- With the help of the neural networks it is possible to obtain a material having desired properties. This method can be applied to new materials development in general, not only to non-flammable mixtures described in this paper.
- A practically applicable, non-flammable material has been developed.

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