COBEM 99
XV Congresso Brasileiro de Engenharia Mecânica
15th Brazilian Congress of Mechanical Engineering
22 - 26 de Novembro de 1999 / November 22 - 26, 1999 Águas de Lindóia, São Paulo,

APPLICATION OF NEURAL NETWORKS IN STEELS' CHEMICAL COMPOSITION DESIGN

Leszek A. Dobrzański
Wojciech Sitek
Silesian University of Technology, Institute of Engineering Materials and Biomaterials
Konarskiego St18A, 44-100 Gliwice, Poland

Abstract. *Designing of the chemical composition of the steel heats having the demanded properties, e.g. the defined shape of the hardenability curve, is the crucial task from the manufacturing point of view. Rapid development of computer science and technology as well as of modern computer tools, artificial intelligence among them, prompts their increasingly common use in different domains of science and technology. There is a great interest in these methods, which seems justified, since they can be applied both to solving novel problems and to dealing with the ones considered classical. For a couple of years, such trends have been present also in the domain of materials engineering. Contemporary software tools, especially methods of artificial intelligence, make it possible to develop the method, presented in the paper, of designing of the chemical composition of constructional alloy steels, which still are one of the basic groups of metallic engineering materials. It lets the designer abandon the classical approach to the material selection according to which one of the catalogued materials has to be selected.*

The paper presents the method of designing of the chemical composition basing on the known and the required shape of the hardenability curve with the use of the dedicated neural networks models.

Keywords: *Neural network, Chemical composition, Steel, Hardenability, Modelling*

1. INTRODUCTION

Materials selection features an important issue in machine design, their parts and tools. Apart from the unequivocal definition of the geometrical features like dimensions and their tolerances, the design definition calls for precise determining of properties like material type, e.g. steel grade, heat treatment state, required working properties. As regard the constructional alloy steels, being still an important group of engineering materials, the required working properties are their mechanical properties, including tensile strength, yield strength, toughness, hardenability and other (Pickering, 1978). When steels are considered, the issue of material selection boils down in practice solely to selection of its grade. The methodology proposed in the work features the development of the commonly used solution in the field of constructional steels selection for machine parts, and makes it possible to define precisely the chemical composition of the steel, from which the given set of mechanical properties is required as a function of the technological or other parameters (Fig. 1). The neural network models are presented as an example of the tool employed to solve this problem, making it possible to design the chemical composition of the steel with required Jominy hardenability curve shape.

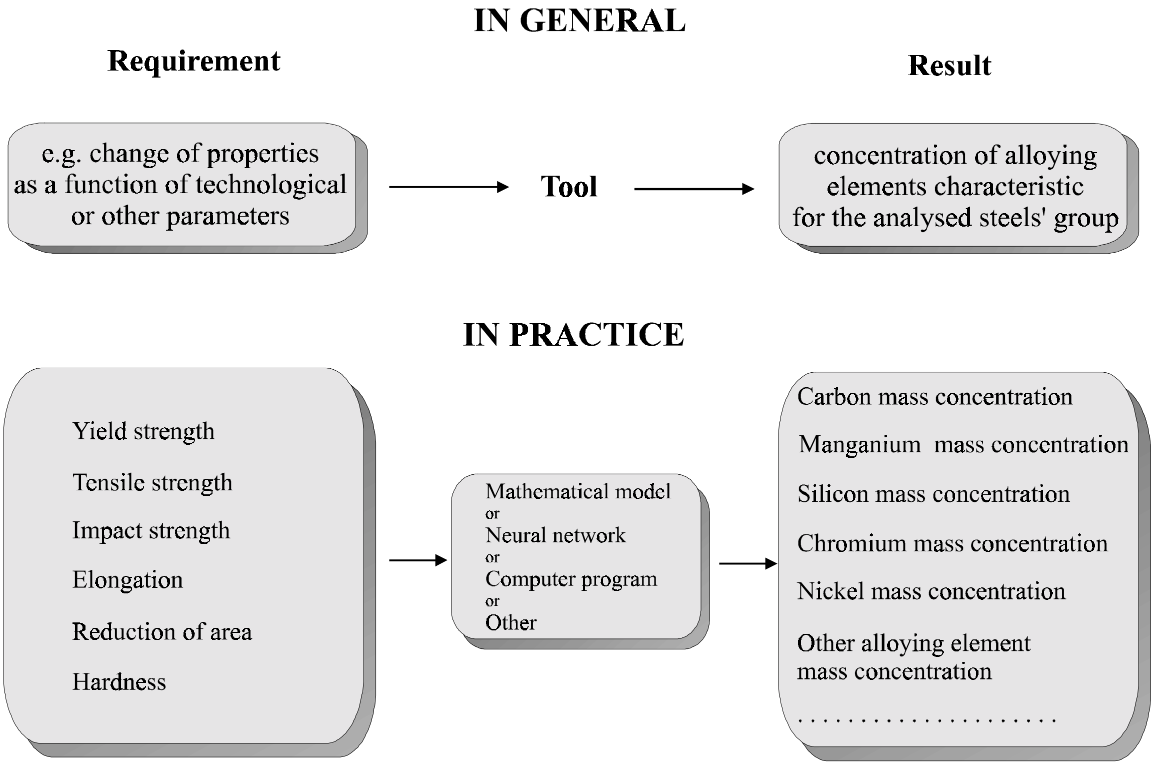

Figure 1 - The flow diagram of modelling the steel chemical composition depending on the defined requirements.

2. MODEL OF THE NEURAL NETWORK FOR DESIGNING OF THE STEELS' CHEMICAL COMPOSITION

The new method is dedicated for the conventional carburising and heat-treatable steels. Carbon, silicon, manganese, chromium, nickel and molybdenum are the main alloying elements used in the carburising and heat-treatable groups of conventional alloy constructional steels considered. The chemical composition calculations were assumed to be made basing on the given hardenability curve shape, presented as the successive hardness values at 15 fixed distances from the Jominy specimen face. Initial classification of steels was done to obtain a high conformity of the computational results with the experimental data. The basis of the classification is the value of the alloy factor (AF) describing digitally the fraction of alloying elements in steel according to standard (ASTM, 1985). The problem is discussed in detail in work (Dobrzański & Sitek, 1998). Basing on the investigations carried out, it was found out that classification of steels into three classes within the framework of each group of carburising and heat-treatable steels is sufficient to obtain a good conformity of the calculations with the experimental data of the chemical composition. Figure 2 presents experimental hardenability bands for each steel group's. Specification of classes of the selected alloy constructional steels' grades and concentration ranges of the basic chemical elements for particular classes are presented in Table 1.

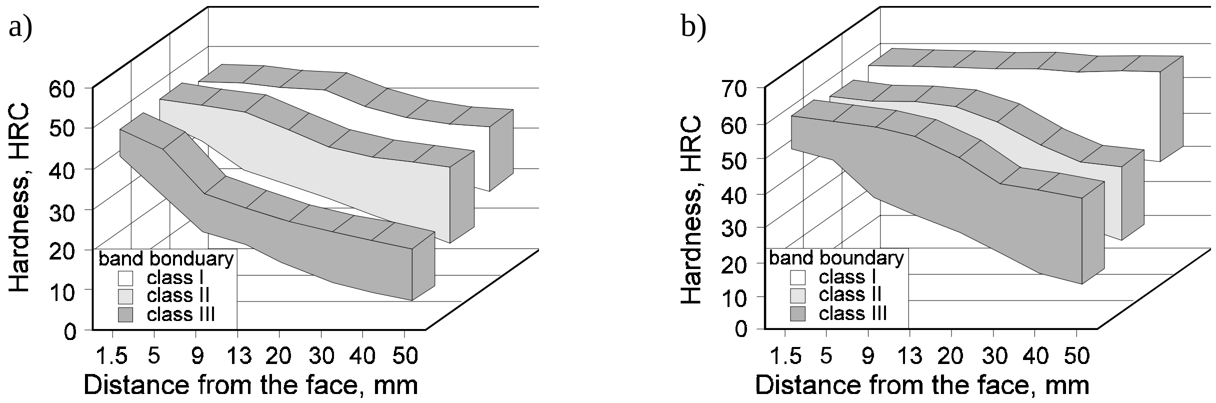

Figure 2 - Experimental hardenability bands for each classes of *a)* carburising steels' and *b)* heat-treatable steels'.

Table 1. Specification of classes of the selected alloy constructional steels' grades and concentration ranges of the basic chemical elements for particular classes.

Steel class		Carburising steels			Heat-treatable steels		
		Class I	Class II	Class III	Class I	Class II	Class III
Steel grade		14CrNi6[1)] 15HN[3)] 17CrNiMo7[1)] 17HNM[3)] 18NiCrMo6[1)]	20HG[3)] 20MnCr5[4)] 5120H[2)] 18HGM[3)] 15HGN[3)]	16MnCr5[1)] 16HG[3)] 18CrMo4[1)] 20NiCrMo2[1)] 20HNM[3)] 8622H[2)] 8625H[2)] 8822H[2)]	35CrNiMo6[1)] 40NiCrMo4[1)] 30HGS[3)] 35HGS[3)] 36HNM[3)] 40HNMA[3)] 4340[2)]	25HM[3)] 30HM[3)] 35HM[3)] 42CrMo4[1)] 709M40[5)] 37HGNM[3)]	34Cr4[1)] 37Cr4[1)] 41Cr4[1)] 40H[3)] 45HN[3)] 30G2[3)] 45G2[3)] 35SG[3)]
Element conentration, wt %	C	0.10-0.20	0.15-0.25	0.13-0.25	0.27-0.48	0.20-0.50	0.27-0.50
	Mn	0.40-0.70	0.80-1.50	0.60-1.30	0.50-1.20	0.40-1.20	0.50-2.00
	Si	0.10-0.35	0.15-0.45	0.15-0.45	max 1.50	max 0.40	0.15-1.50
	Cr	1.25-1.90	0.80-1.40	0.35-1.10	0.50-1.80	0.35-1.30	max 1.25
	Ni	1.30-1.85	max 0.35	max 0.65	max 2.00	max 0.80	max 1.30
	Mo	max 0.35	max 0.30	max 0.30	max 0.35	0.10-0.30	max 0.10

1) according to EN standards
2) according to SAE/AISI standards
3) according to PN standards
4) according to DIN standards
5) according to BS standards

For designing of the chemical composition of the steel with the required hardenability, unidirectional multilayer neural networks were employed with the learning method based on the error backpropagation algorithm. Fifteen input nodes and 6 output ones assumed in the network structure are the consequence of the assumption that the hardenability of the steels' analysed is affected mainly by the concentration of six basic alloying elements. And additionally, hardenability curve is plotted by the values of hardness measured at fifteen successive points in fixed distances from Jominy specimen face. Finally, after preliminary tests, the 15-30-6 network model (Fig. 3) was assumed for the calculations, with the learning coefficient η=0.15 and momentum parameter α=0.3.

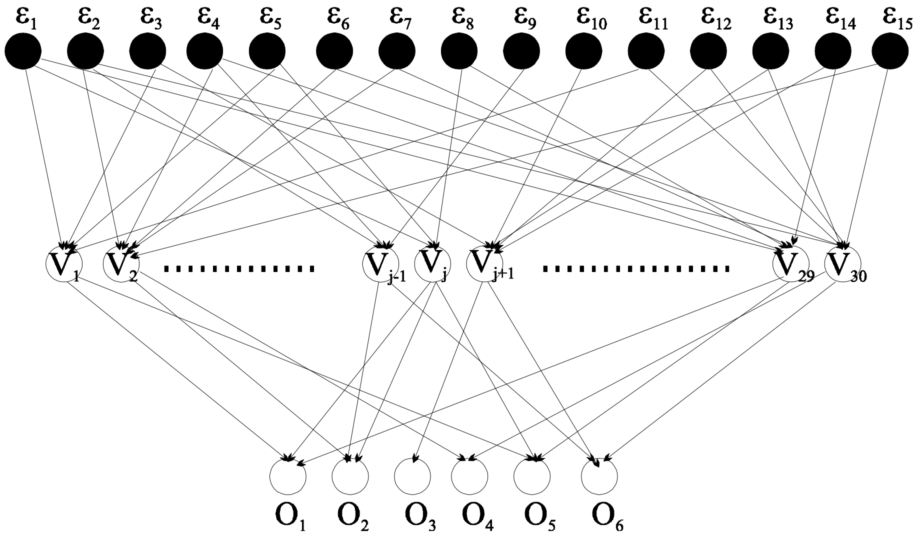

Figure 3 - Model of the neural network employed for the designing of the chemical composition of steel (ε_i – input nodes, v_i – hidden nodes, o_i – output nodes).

Networks with such structures were trained individually for each steel class, using a data set prepared basing on the results of the experiments carried out. The neural networks developed were experimentally verified, which consisted in the evaluation of the conformity of the computational results (obtained by using the network models) with the experimental data. As a criterion of the evaluation a coefficient of assessment of the computation method adequacy *s* was employed. The coefficient defines the difference between the required hardenability and the one obtained for an actual heat. As a result of the investigations performed, the limiting value 2.5 HRC of the coefficient *s* was assumed (Dobrzański & Sitek, 1998).

3. VERIFICATION OF THE NEURAL NETWORK MODELS

Verification procedure for such a model consists in calculating the chemical composition of the steel with the required Jominy curve shape and in making the heat of the steel with the chemical composition calculated. Then, the relevant hardenability investigation is carried out and the actual experimental hardenability curve of the heat is compared to the required Jominy curve shape. For experimental verification hardenability curves with the assumed and distinctly different shapes were selected. Calculations of the chemical composition for the curves with the required shape were made within the framework of a particular steel grade only when the required hardenability curve was within the experimental hardenability band for the class considered. Then, investigations of hardenability of the heats with the actual chemical compositions the nearest to the calculated ones were made. Hardenability curves' shapes, the required and the actual ones, were compared afterwards. As an example of the calculations made, the results for two of the required shapes of hardenability curves are presented (curve No. 1 for carburising steel, curve No. 2 for heat-treatable steel). The chemical compositions calculated within the framework of each steel class for which the required hardenability curve is within the experimental hardenability band and the relevant chemical compositions of the actual heats are included in Table 2. Figure 4 presents the graphical comparison of the required hardenability curve and the experimental ones for the steel heats with the designed chemical composition.

Table 2. Comparison of the calculated and the relevant chemical compositions of the actual heats

Required curve shape	Chemical composition	Concentration of the alloying elements, wt %					
		C	Mn	Si	Cr	Ni	Mo
1	calculated	0.20	0.91	0.29	0.93	0.12	0.25
	actual I	0.18	0.95	0.28	0.95	0.12	0.23
	calculated	0.24	0.80	0.26	0.59	0.53	0.32
	actual II	0.23	0.78	0.29	0.53	0.45	0.32
	calculated	0.22	0.59	0.23	1.01	0.18	0.22
	actual III	0.26	0.6	0.2	1.06	0.16	0.21
2	calculated	0.41	0.60	0.25	0.75	1.29	0.16
	actual I	0.41	0.68	0.28	0.74	1.35	0.16
	calculated	0.40	0.77	0.29	1.01	1.29	0.18
	actual II	0.40	0.72	0.31	1.03	1.35	0.17
	calculated	0.42	0.79	0.26	1.02	0.23	0.07
	actual III	0.41	0.69	0.36	1.06	0.26	0.07

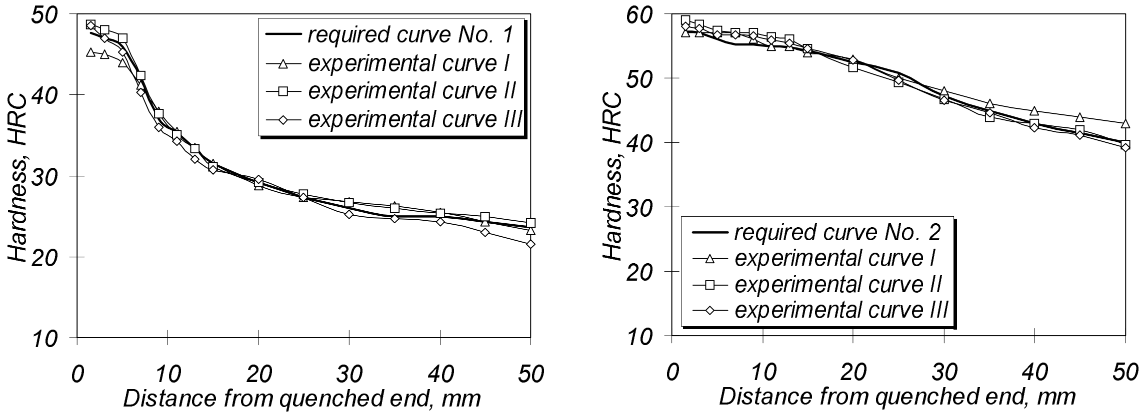

Figure 4 - Comparison of the required hardenability curves and the experimental ones of the steels' heats of the designed chemical composition

Basing on such calculations made for about 550 testing industrial heats it was found out that the neural network model developed secures the satisfactory adequacy with experimental data since in each case the calculated coefficient of adequacy assessment *s* is smaller than its critical value 2.5 HRC (Table 3).

Table 3. The average value of the coefficient of the methods' adequacy *s* obtained for each steels' class

Steels' group					
Carburizing steels			Heat-treatable steels		
Class I	Class II	Class III	Class I	Class II	Class III
1.4	2.2	1.6	1.8	1.6	2.2

4. REMARKS

The adequate models of the relations between the hardenability and the chemical composition of the alloy constructional steels, using the neural networks were developed. The method of designing of the steel chemical composition basing on the required hardenability curve shape was presented in the paper. The model was then experimentally fully verified. All generalizations are based on the vast set of the experimental data. The results of the tests carried out on about 450 heats were taken for neural networks' training in the case of each model. About 550 heats of the carburising and heat-treatable steels with various chemical compositions were used for testing. The developed method of designing of the steel chemical composition basing on the knowledge of Jominy hardenability curve shape is useful in practice, e.g. for the real-time control of the chemical composition of the steel with the strictly demanded hardenability curve shape during the heating process

5. ADDITIONAL INFORMATION

The investigations were partially carried out within the framework of the research project of the Committee of Scientific Research (Poland) No 7 T08A 07412 headed by prof. L.A. Dobrzański.

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