

YEAR XI **Issue 12** / 2017 **ISSN PRINT 1313-0226**
ISSN WEB 1314-507X

International journal
for science, technics and
innovations for the industry



MACHINES
TECHNOLOGIES
MATERIALS



Published by
Scientific technical
Union of Mechanical Engineering "INDUSTRY 4.0"



MACHINES. TECHNOLOGIES. MATERIALS

INTERNATIONAL SCIENTIFIC JOURNAL

PUBLISHER

SCIENTIFIC TECHNICAL UNION OF MECHANICAL ENGINEERING “INDUSTRY 4.0”

108, Rakovski Str., 1000 Sofia, Bulgaria

tel. (+359 2) 987 72 90,

tel./fax (+359 2) 986 22 40,

office@stumejournals.com

www.stumejournals.com

ISSN PRINT 1313-0226, ISSN WEB 1314-507X, YEAR XI, ISSUE 12 / 2017

EDITOR-IN-CHIEF

Prof. D.Sc. DHC Georgi Popov,

President of Bulgarian Scientific and Technical Union of Mechanical Engineering

EDITORIAL BOARD

MEMBERS

SCIENTIFIC COMPETENCE

Prof. Dimitar Damyanov	Automatisation of production
Prof. Dimitar Karaivanov	Mechanics of machines
Prof. Dimitar Stavrev	Technologies and materials
Prof. Dimitar Yonchev	National and industrial security
Prof. Galina Nikolcheva	Machines tools and technologies
Prof. Hristo Shehtov	Automatisation of production
Prof. Idilija Bachkova	Automatisation of production
Prof. Ivan Kralov	Mechanics of machines
Prof. Ivan Parshorov	Technologies and materials
Prof. Ivan Yanchev	Machines and technologies
Prof. Ivo Malakov	Automatisation of production
Prof. Kiril Angelov	Industrial Management
Prof. Lilo Kunchev	Transport Equipment and Technology
Prof. Lubomir Dimitrov	Machines and technologies
Prof. Miho Mihov	Agricultural machinery
Prof. Miroslav Denchev	Ergonomics and design
Prof. Mladen Velez	Economics and Marketing
Prof. Nikolay Diulgerov	Technologies and materials
Prof. Ognyan Andreev	Production management
Prof. Petar Kolev	Transport Equipment and Technology
Prof. Roman Zahariev	Robotics
Prof. Sasho Guergov	Robotic systems and technology
Prof. Tsanka Dikova	Technologies and materials
Prof. Vitan Galabov	Mechanics of machines



MACHINES. TECHNOLOGIES. MATERIALS

INTERNATIONAL SCIENTIFIC JOURNAL

ISSN PRINT 1313-0226, ISSN WEB 1314-507X, YEAR XI, ISSUE 12 / 2017

EDITORIAL BOARD FOREIGN MEMBERS

Prof. Adel Mahmoud	IQ	Prof. Marian Tolnay	SK
Prof. Ahmet Ertas	TR	Prof. Mark Easton	AU
Prof. Andonaq Londo	AL	Prof. Mart Tamre	EE
Prof. Andrei Firsov	RU	Prof. Maryam Ehteshamzade	IR
Prof. Andrzej Golabczak	PL	Prof. Michael Evan Goodsite	DK
Prof. Anita Jansone	LV	Prof. Movlazade Vagif Zahid	AZ
Prof. Aude Billard	CH	Prof. Natasa Naprstkova	CZ
Prof. Bojan Dolšak	SI	Prof. Oana Dodun	RO
Prof. Christian Marxt	LI	Prof. Oleg Sharkov	RU
Prof. Dale Carnegie	NZ	Prof. Páll Jensson	IS
Prof. Ernest Nazarian	AM	Prof. Patrick Anderson	NL
Prof. Esam Husein	KW	Prof. Paul Heuschling	LU
Prof. Ewa Gunnarsson	SW	Prof. Pavel Kovac	RS
Prof. Filipe Samuel Silva	PT	Prof. Per Skjerpe	NO
Prof. Francisco Martinez Perez	CU	Prof. Péter Korondi	HU
Prof. Franz Haas	AT	Prof. Peter Kostal	SK
Prof. Genadii Bagliuk	UA	Prof. Juan Alberto Montano	MX
Prof. Georg Frey	DE	Prof. Raul Turmanidze	GE
Prof. Gregory Gurevich	IL	Prof. Renato Goulart	BR
Prof. Haydar Odinaev	TJ	Prof. Roumen Petrov	BE
Prof. Hiroyuki Moriyama	JP	Prof. Rubén Darío Vásquez Salazar	CO
Prof. Dr. Ilir Doci	Ko	Prof. Safet Isić	BA
Prof. Iryna Charniak	BY	Prof. Sean Leen	IE
Prof. Ivan Svarc	CZ	Prof. Shi Xiaowei	CN
Prof. Ivica Veza	HR	Prof. Shoirdzan Karimov	UZ
Prof. Jae-Young Kim	KR	Prof. Sreten Savićević	ME
Prof. Jerzy Jedzejewski	PL	Prof. Stefan Dimov	UK
Prof. Jean-Emmanuel Broquin	FR	Prof. Svetlana Gubenko	UA
Prof. Jordi Romeu Garbi	ES	Prof. Sveto Cvetkovski	MK
Prof. Jukka Tuhkuri	FI	Prof. Tamaz Megrelidze	GE
Prof. Katia Vutova	BG	Prof. Tashtanbay Sartov	KG
Prof. Kazimieras Juzėnas	LT	Prof. Teimuraz Kochadze	GE
Prof. Krasimir Marchev	USA	Prof. Thorsten Schmidt	DE
Prof. Krzysztof Rokosz	PL	Prof. Tonci Mikac	HR
Prof. Leon Kukielka	PL	Prof. Vasile Cartofeanu	MD
Prof. Mahmoud El Gammal	EG	Prof. Yasar Pancar	TR
Prof. Manolakos Dimitrios	GR	Prof. Yuriy Kuznetsov	UA
Prof. Marat Ibatov	KZ	Prof. Wei Hua Ho	ZA
Prof. Marco Bocciolone	IT		

CONTENTS

MACHINES

MODEL FOR DETERMINING THE STATIC LOAD ON MOVABLE SPATIAL CONSOLE LATTICE GIRDER BOUNDED WITH CLAMPS Prof. Dr. Sc. Hristovska E., mech. eng., Assis. Prof. Dr. Sc. Sevde Stavreva, Prof. Dr. Sc. Vangelica Jovanovska, Assoc. Prof. Dr. Sc. Ivo Kuzmanov, Assoc. Prof. Dr. Sc. Zlatko Sovreski	551
--	-----

TECHNOLOGIES

PROVIDING MECHANICAL CHARACTERISTICS OF WELDING-SOLDERED THIN-WALLED STRUCTURES OF MULTICOMPONENT HEAT-RESISTANT ALLOYS Prof. Dr. Eng. Salenko O., Prof. Ph. D. Eng. Shchetynin V., Lashko E., Ph. D. Eng. Potapov O., Ph. D. Eng. Gusarova I.	554
IMPACT OF THE DECARBURIZATION LAYER ON THE CRACK PROPAGATION IN HIGH FREQUENCY WELDED JOINT Prof. Dr. Maksuti Rr.	558
MODELING AND SIMULATION OF INDUSTRIAL PROCESSES Christo Boyadjiev	562
SIMULATION OF THE PROCESSES OF ENCODING AND DECODING WITH LINEAR BLOCK CODES DETECTING AND CORRECTING ERRORS Assist. Prof. M.Sc. Borodzhieva A. PhD., M.Sc. Aliev Y., Assoc. Prof. M.Sc. Ivanova G. PhD	566
ELECTRIC POWER SYSTEMS MODELING AND EDUCATION: SHORT TERM UNIT COMMITMENT AND ECONOMIC DISPATCH MODELING FRAMEWORK M.Sc. Trashlieva V., M.Sc. Radeva T. PhD.	572
ROBUST DESIGN AND MULTIPLE CRITERIA OPTIMIZATION OF ELECTRON BEAM GRAFTING OF CORN STARCH Assoc. Prof. M.Sc. Eng. Koleva E. PhD., M.Sc. Eng. Koleva L., M.Sc. Eng. Nemțanu M.R. PhD., M.Sc. Brașoveanu M. PhD.	575
TRAFFIC AND DRIVERS SYMBIOSIS: MANAGING BOTH FOR LOWER AIR POLLUTION assistant professor dr. Angelevska B., full professor Markoski A., full professor dr. Atanasova V.	579
TRAFFIC PRODUCTION MODEL USING MULTIPLE REGRESSION ANALYSIS AND RADIAL BASIS FUNCTION NEURAL NETWORK Prof.dr.Vaska Atanasova., Mr.sc. Ramadan Duraku., Associate prof.dr Beti Angelevska , Prof.dr.Nikola Krstanoski.	583
 <u>MATERIALS</u>	
APPLICATION OF CAD DESIGN OF TECHNOLOGICAL PROCESSES IN THE FIELD OF MATERIAL SCIENCE Emil Hr. Yankov, Nikolay Tontchev, Simeon Yonchev	587
SURFACE MORPHOLOGY AND WETTABILITY OF GRADIENT (Ti,Al,V)N/TiO₂ COATING Nikolova M. PhD.	591

MODEL FOR DETERMINING THE STATIC LOAD ON MOVABLE SPATIAL CONSOLE LATTICE GIRDER BOUNDED WITH CLAMPS

Prof. Dr. Sc. Hristovska E., mech. eng.¹, Assis. Prof. Dr. Sc. Sevdie Stavreva¹, Prof. Dr. Sc. Vangelica Jovanovska²,
Assoc. Prof. Dr. Sc. Ivo Kuzmanov¹, Assoc. Prof. Dr. Sc. Zlatko Sovreski¹

¹Faculty of Technical Sciences – Bitola, University St. Kliment Ohridski, Republic of Macedonia

²Faculty of Biotechnical Sciences – Bitola, University St. Kliment Ohridski, Republic of Macedonia

elizabetha.hristovska@uklo.edu.mk

Abstract: This paper presents a model for determining the static load on movable spatial console lattice girder and the clamps which bounded the same one. The paper presents guidelines for theoretical determination of the static load using an appropriate software package and conducted modeling for this purpose. Also, the paper displays the methodology for experimental determining the static load by setting a model for the experimental measurement on the specific measuring points of the clamps and the characteristic positions of the carrying console. The research is carried out on a concrete real object and the results are shown numerically and graphically, which enables carrying out an analysis of the load and deducing concreting conclusions about the research object.

Keywords: CARRYING CONSOLE, CLAMPS, STATIC LOAD, THEORETICAL DETERMINATION, EXPERIMENTAL MEASUREMENT

1. Introduction

The carrying construction of the working wheel on a rotating excavator is a spatial steel console bounded with clamps, which can be moved in a horizontal and vertical plane. In the horizontal plane, moving this console is enabled by turning the lower construction of the excavator. In the vertical plane, the moving is from nethermost position where digging is below the ground level to the uppermost position at the maximum digging height above the ground level.

The spatial carrying console is with a lattice design, which at its first end is jointly connected, and at the free end carries the working (rotating) wheel of the excavator. The console is bounded with two clamps, usually with a rectangular cross-section, which with the opposite ends are carried on to the upper construction of the counterweight of the excavator (ballast construction).

The static load of the clamps of this spatial console lattice girder is by its own weight from the construction that they hold, and theoretically these are the load sizes for the standby condition of the excavator. In particular, the static loads of the clamps are tensile forces as a reaction from the weights of the elements on the working wheel and its carrying construction.

The static load of the clamps can be determined by theoretical and experimental way. The theoretical determination is based on a static calculation of the forces in the clamps using the static balance conditions for the three characteristic positions of the carrying console - uppermost, horizontal and nethermost position. The experimental determination is based on an experimental measurement of the forces in the clamps, at measuring spots (points) in the most loaded cross-section of the clamps, for the characteristic positions of the carrying console.

2. Theoretical determination of the static load

For theoretical determination of the static loads onto the clamps, it is necessary to set up the model of the carrying console and its clamps. The mathematical (numerical) model needs to implement a computer static calculation, and the same one should be close to the real model.

For a concrete rotating excavator, the excavator SRs-630/I product of the German company TAKRAF, which works in the coalmine "Suvodol" Bitola, sets the real and mathematical model of the carrying console and its clamps (Figure 1 and Figure 2).

Knowing the technical characteristics of the construction and application of a matrix analysis of the construction with a software package for this purpose, the static loads for the characteristic positions of the load carrying construction are determined, or loads on the excavator's standby without taking into account the working conditions.

The theoretical (analytical) determination of the static loads on the clamps of the rotating excavators finds justification in the development phase of the excavators (even when there is no real object) because it is a faster and cheaper way but with less accuracy than the experimental determination.

Calculated sizes of forces in the clamps which come from static load, using the SAP 2000 software package, are listed in Table 1.

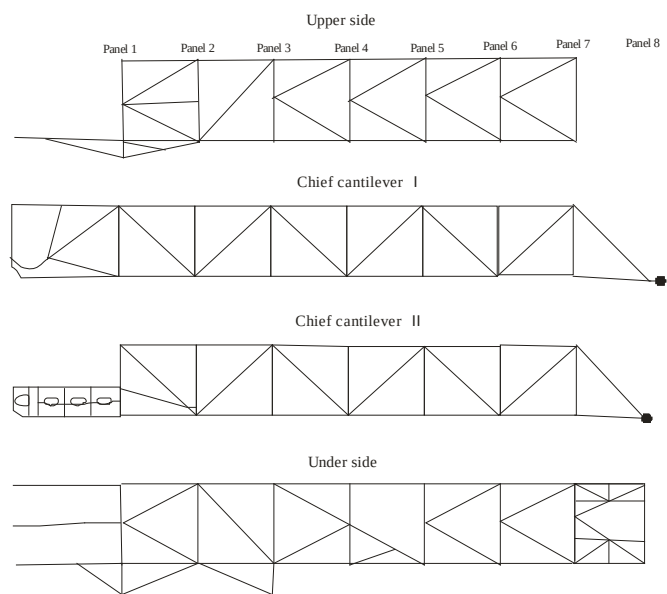


Fig. 1 Real model of the carrying console

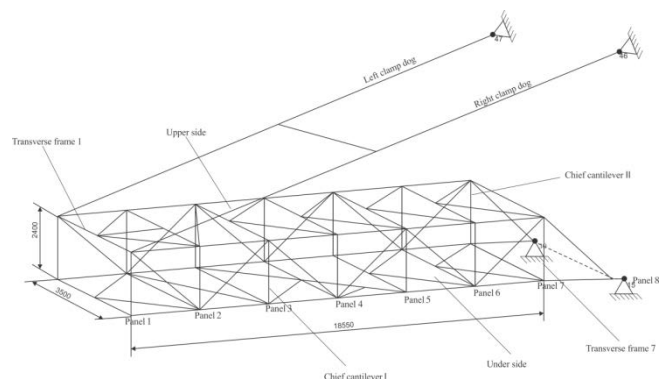


Fig. 2 Mathematical model of the carrying console and its clamps

Table 1. Theoretical sizes of forces from static load

Position of carrying structure	Tension force in [kN]	
	Right clamp	Left clamp
Uppermost	773.13	748.01
Horizontal	850.32	823.39
Nethermost	819.47	792.92

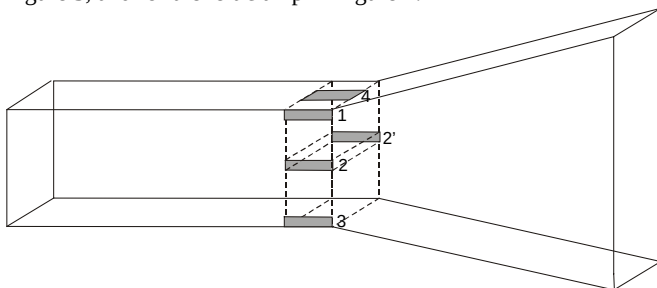
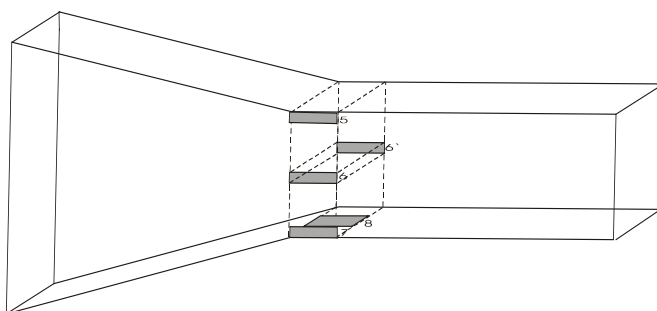
3. Experimental determination of the static load

The experimental determination of the static loads on the clamps of the carrying consoles could be done by measuring the strains to which they are exposed when the excavator is on standby, for characteristic positions of the console. The strains in excavator standby position are reaction to the own weight of the structural elements.

Stresses measurement of clamps is carried out in an indirect way, or by measuring the dilatations at certain measuring spots of the clamps with the most used method for this purpose - the tensiometric method. The dilatations of the measuring points are measured with the set measuring strain gages, and the connection of the dilatations with stresses and stresses with loads should be established using certain settings of the materials strength.

The measurement of the static loads of the two clamps on the carrying console of the rotating excavator working wheel requires a longer and more difficult preparation, given the working conditions of the excavator which is carried out according to a conceptual methodology for this purpose.

For the measurements of the excavator SRs-630 onto the both clamps there are placed five measuring gages for measuring axial stresses, with different layout on each clamp. The measuring gages on the two clamps are placed in the intersection, which according to the estimation is considered to be the most overloaded, and is located at the transition from the constant cross-section of the clamps toward the tilt, where the clamps with the little axles are joined to the carrying console of the excavator's wheel. The arrangement of the measuring gages for the right clamp is shown in Figure 3, and for the left clamp in Figure 4.

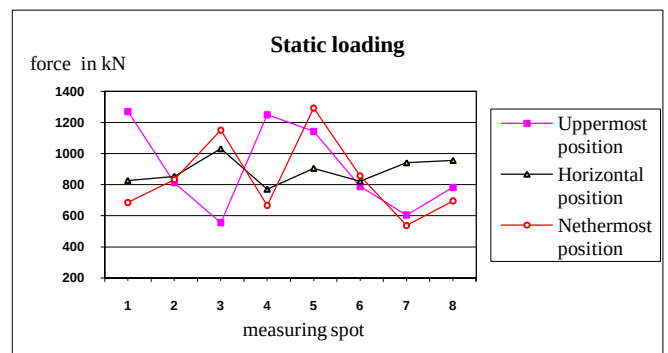
**Fig. 3** Measuring gages on the right clamp, with an inside view**Fig. 4** Measuring gages on the left clamp, with an inside view

The measured sizes of loads from the static load, at each of the measuring points (spots) of the both clamps are shown in Table 2 for the three characteristic positions of the carrying console on the excavator's working wheel.

Table 2. Experimental sizes of forces from static load

Position of carrying structure	Magnitude of force from static load in [kN]							
	Right clamp				Left clamp			
	Measuring point				Measuring point			
	1	2	3	4	5	6	7	8
Uppermost	1270.08	812.45	555.31	1248.91	1141.9	788.26	604.65	782.01
Horizontal	826.56	853.07	1031.28	770.16	904.93	822.53	940.56	955.79
Nethermost	685.44	832.76	1150.28	666.09	1292.76	856.80	537.47	695.12

In order to obtain a clearer picture of the measurement magnitudes obtained by the experimental measurement, all the final results of the performed measurements are processed and systematized and the diagrammatic shown in Figure 5.

**Fig. 5** Static load on the clamps for the characteristic positions of the carrying console

4. Measurement characteristics

The static load of the clamps was measured by the following way: the carrying structure of the working wheel was leaning in a lower position at rest, on supports with hydraulic pumps, in which position the clamps were loosened, or unloaded. This condition is the conditional zero of the load on the clamps. The carrying console is raised by about 2 m and the static load on both clamps is measured for a horizontal position. The carrying console was then lifted up to its uppermost position, for which position the static load of the clamps was measured. The static load on the clamps was also measured for the nethermost position of the carrying console on the working wheel.

During the measurement, the static load change in the clamps was followed from the influence of:

- removal of the hydraulic support of the carrying console;
- turning the console left and right ;
- turning the working wheel without load;
- the work of the conveyor tape on the carrying console without load;
- the transport of the excavator.

From all previously mentioned the following conclusion is ascertained:

The extraction of hydraulic supports does not cause a change in the static load on the right clamp, while in the left this change is small by increasing on the measuring spot 6 and decreasing on the measuring spot 7.

When turning the carrying console to the right, change in the load on the right and left clamp is recorded. On the right clamps - the measuring spot 1 and 4 have a lower force, which is 62% and 59% respectively of the load size in this position of the console before the turning starts; at the measuring spot 3, an increase of 69% of the load before turning; no change in load was recorded at measuring spot 2. On the left clamp - at the measuring spot 5 there is a 38% reduction in the load; on measuring spots 7 and 8 there is an increase of 100%; while no change has been recorded at measuring spot 6.

When turning the carrying construction to the left it is recorded for the two clamps the same load change at measuring spots as when turning to the right, but with some smaller forces.

The rotating of the working wheel without load does not cause a change in the load condition of the clamps.

The work of the conveyor tape without load does not cause a change in the load on the clamps.

The transport of the excavator also does not cause a significant change in the load. Negligible oscillatory load changes are recorded at measuring spot 3 on the right clamp and measuring spot 6 on the left clamp.

5. Conclusion

The theoretical determination results of the static loads on the clamps of carrying console should be treated as orientation values because they do not take into account the specific working environment impacts and the actual technical condition of the excavator, as well as the change in the size of the forces at different positions at the cross-section of the clamps.

The experimental determination results of the static loads on the clamps of carrying consoles are relevant for further analysis. The analysis of the results of the experimental measurement showed that the relevant sizes for the loads of the clamps are the measured forces at the neutral axis of the cross-section of the clamp (measuring spot 2 at the right and the measuring spot 6 on the left clamp).

The static loads of the clamps are the largest for the horizontal position of the carrying console, with the note that the load on the right clamp is greater.

The display on the same diagram of the measured forces for the two clamps per measuring spots and positions of the carrying console allows us to perceive the difference in the load sizes of the two clamps for the same position of the carrying console, for all measuring spots, as well as the difference in the load per measuring spots for the characteristic positions of the console.

6. References

- [1] Hristovska, E., Characteristic of the working load on the rotating excavator, 8th International Conference "Machinery, technology, materials", Sofia, Bulgaria, 2010.
- [2] Hristovska, E. etc., Measurement and testing of loads and stress deformed state of the carrying construction of the excavator SRs-630/1 in the coalmine Suvodol-Bitola, Application project, Faculty of Mechanical Engineering-Skopje, Macedonia
- [3] Hristovska, E. etc., Analysis of the stability of the excavator SRs-630 with the reconstruction of the working wheel, Application project, FAKOM engineering-Skopje in cooperation with Faculty of Technical sciences-Bitola and Faculty of Mechanical Engineering-Skopje, Macedonia
- [4] Operating instructions for the excavator SRs-630 and other technical documentation for this excavator, REK-Bitola
- [5] Technical documentation from the excavator SRs-630 manufacturer, TAKRAF-Germany

PROVIDING MECHANICAL CHARACTERISTICS OF WELDING-SOLDERED THIN-WALLED STRUCTURES OF MULTICOMPONENT HEAT-RESISTANT ALLOYS

ОБЕСПЕЧЕНИЕ МЕХАНИЧЕСКИХ ХАРАКТЕРИСТИК СВАРОЧНО-ПАЯНЫХ ТОНКОСТЕННЫХ КОНСТРУКЦИЙ ИЗ МНОГОКОМПОНЕНТНЫХ ЖАРОСТОЙКИХ СПЛАВОВ

Prof. Dr. Eng. Salenko O.¹, Prof. Ph. D. Eng. Shchetynin V.², Lashko E.³,
Ph. D. Eng. Potapov O.⁴, Ph. D. Eng. Gusarova I.⁵

Kremenchuk Mykhailo Ostrohradskyi National University^{1,2,3}, Yuzhnoye Design Office^{4,5} – Kremenchuk, Dnipro, Ukraine

evgeny.lashko.lj@gmail.com

Abstract: The main task of the research is to establish the regularities of the formation of a non-detachable compound of thin-walled elements from the Ni-20Cr-6Al-1Ti-1Y2O3 alloy and to determine the functional condition of the influence of soldering modes on the physical-mechanical characteristics of the compound. It has been shown the modeling of temperature fields in ANSYS 18.1. It has been established that the process of vacuum soldering should take place at a temperature of 1350°C for 15-20 min; the strength of the resulting compound is 390-420 MPa when the sample is stretched. The obtained information can be used as a theoretical basis for the development of the manufacturing process of the elements of the spaceship heat-shielding system.

KEYWORDS: WELDING; SOLDERING; HEAT TRANSFER; VACUUM; HEAT-RESISTANT MULTICOMPONENT ALLOYS

1. INTRODUCTION

Heat-resistant multicomponent alloys, in particular Ni-20Cr-6Al-1Ti-1Y2O3, are used in special engineering, since they successfully withstand the effects of high temperatures (up to 1100-1200°C), while retaining satisfactory strength, bending linear hardness, other important mechanical characteristics.

Studies aimed at developing ways and methods for obtaining non-detachable compounds (eg, diffusion welding, soldering in vacuum, contact welding on a previously applied substrate), show that the most qualitative for today is diffusion welding in vacuum. The latter involves the creation of not only the high temperatures necessary to activate the diffusion process between the interconnected surfaces, but also significant pressures at the point of contact (up to 50-75 MPa), which, as a rule, are provided, due to the temperature expansion of connected elements those which are enslaved in a special equipment. Typically, such elements are firm and solid specimens, that withstand specified pressures without significant deformations, which lead to errors in the shape of the finished product.

The preparation of specimens, which are spatial non-rigid elements that contact several planes of a small area, did not succeed in this way, which requires the search for methods and techniques for carrying out similar operations with simultaneous optimization of the stiffness parameter of the seam and the absence of significant thermal deformations. An example of products that require the assembly of individual elements in a single design, is a three-layer cellular panel, used, for example, as the re-usable thermal protection of a space vehicle.

The multicomponent Ni-20Cr-6Al-1Ti-1Y2O3 alloy is sufficiently investigated by scientists and technical specialists [1-3], with some papers indicating that the alloy is satisfactorily exposed to diffusion welding and welding-soldering [1].

At the same time, it is noted that the traditional technologies of formation of an indivisible connection of thin plates by loading the junction zone with the nickel-based solder on the basis of nickel with stresses of 35-70 MPa with a subsequent shut-off at a temperature of 1250-1350°C for 15-20 minutes in a vacuum are ineffective. The reason lies in the fact that places for soldering of heat-protective elements are difficult to access; elements and systems of the cellular panels are not rigid, and it is practically impossible to provide such a level of prior compression of surfaces.

2. EXPOSITION

Suppose you want to connect two flat elements on the surface, which is a thin strip (fig. 1).

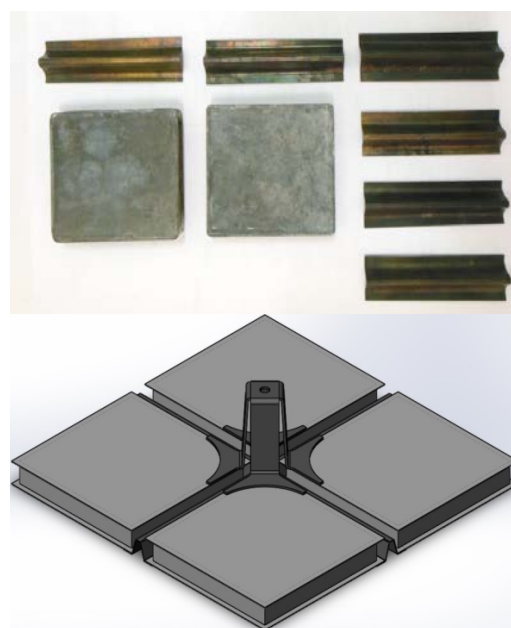


Fig. 1. The unit that is exposed to soldering in a vacuum and its calculation scheme

To ensure reliable welding of plates, two conditions must be fulfilled:

- the pressure between the welded plates should be at least p_{min} ;
- the temperature of the connection place should be $T_n=1330-1350^\circ\text{C}$ and be uniform throughout the length of the seam.

Variation of temperature can lead to incomplete soldering or to the appearance of burning and reflow zones.

Since the connection is performed in a vacuum, the heating of the welding zone is mainly due to heat radiation and, to a lesser extent, due to the contact of one of the welded elements with a heated base.

It is known that the amount of energy emitted by a surface element dF , oriented at a spatial angle $d\Omega$ and φ - the angle between the direction of radiation and the normal to the surface, will be determined as:

$$dQ_\varphi = E_n d\Omega dF \cos \varphi, \quad (1)$$

where $E_n = 4,9 \frac{\varepsilon}{\pi} \left(\frac{T}{100} \right)^4$; ε – the degree of blackness of the

radiating body; then $dQ_\varphi = 4,9 \frac{\varepsilon}{\pi} \left(\frac{T}{100} \right)^4 d\Omega dF \cos \varphi$.

Since the heated body has a sufficient length, the temperature regime at each particular point can be determined by the third-generation boundary conditions.

$$\lambda \frac{\partial T(M, t)}{\partial n} \bar{l}_n = \sigma (T_2^4 - T_1^4(M, t)), \quad (2)$$

where σ – constant Stefan-Boltzmann: $\sigma = 5,67 \times 10^{-8} \text{ W}/(\text{m}^2 \text{ K}^4)$; $\bar{l}_n$ – vector normal to the surface of the body; λ – coefficient of thermal conductivity of the absorbing body.

Simultaneously with the transfer of heat by radiation, the specimen will receive heat and from the base on which it is located, which is determined by the boundary conditions of the 4th genus:

$$\lambda \frac{\partial T(M, t)}{\partial n} \bar{l}_n = \lambda_2 \frac{\partial T_2(M, t)}{\partial n} \bar{l}_n, \quad (3)$$

where λ_1, λ_2 – the coefficient of thermal conductivity of the absorbing and radiating body, respectively.

The simplified amount of transferred heat Q_Σ from the N heating lamellae of the vacuum chamber, taking into account the partial reflection from the body, which is heated, predetermined ε , can be defined as:

$$Q_\Sigma = Q_k + NQ_z - Q_o = \frac{\lambda}{H} ts(T_1 - T_2) + N\gamma s\sigma T_1^4 - F\omega \cos \beta \varepsilon \sigma T_1^4, \quad (4)$$

where φ – coefficient of «not blackness», ω – the corporal angle in which radiation occurs, β – the angle between the direction of radiation and the normal to the surface.

For a cylindrical coordinate system, the temperature change T on the surface of the plate, which receives heat by radiation from heaters:

$$\frac{\partial T_1}{\partial n} = \alpha \nabla^2 T_1 + \frac{q}{c\rho}, \quad \nabla^2 T_1 = \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{1}{r^2} \frac{\partial^2 T}{\partial \varphi^2} + \frac{\partial^2 T}{\partial z^2}.$$

Here r, φ and z – radial, angular and axial coordinates respectively.

An increase in the temperature of a specimen causes its thermal expansion, which for a plate is defined as follows: $\Delta l = \alpha T l_0$ then the emerging stresses with a solid latching of plate will be: $\sigma_t = \alpha E T$.

Since the heating of the plate occurs with several lamellae, located around the base at a certain distance, and the plate itself is on the heat insulating surfaces, it is quite difficult to obtain a picture of the temperature deformations in general. To solve this problem, and taking into account the configuration of the body, which is heated, perform modeling of temperature fields in ANSYS 18.1. Let's take into account the real design features of the used vacuum equipment: the diameter of the platform for installation 320 mm; plate dimensions 75×75 mm; plate thickness $h_1=0,4$ mm; $h_2=0,14$ mm. The soldered elements are located on ceramic plates in the thickness of 7,5 mm; the thermal conductivity of which is much less than the thermal conductivity of the base and the soldered elements.

The transition from the plate to the assembled cellular structure requires taking into account the temperature change in height and on the surface of the heated body. In order to prevent the overheating of the cellular structure during the soldering, thermal ballasts in the form of heat sinks made of solid alloy are installed on the table. Their diameter is $d_b=35$ mm, $h_b=50$ mm.

Figure 2 shows the results of calculations of the thermal field at the time of heating end and the picture of thermal radiation of elements that are on the table.

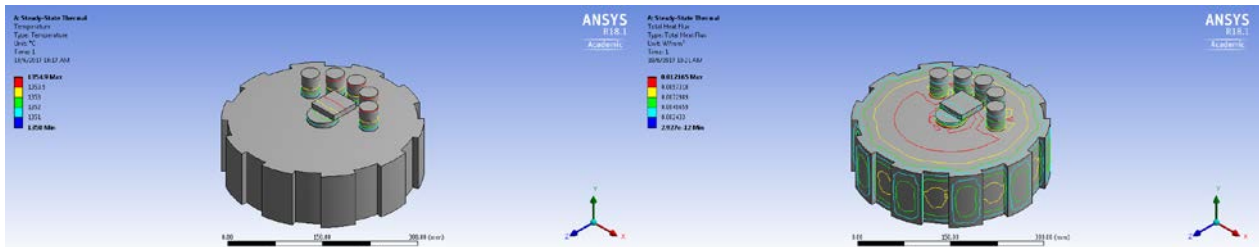


Fig. 2. Temperature fields and radiation of heated bodies in the chamber of vacuum furnace

It is shown that on the plate the temperatures are distributed unevenly, which will result the hogging of the plate or the structure as a whole. It is possible to reduce deformation of elements by using clamping plates, the mass m_p of which should be sufficient to prevent hogging, and at the same time, not cause significant deformations of the construction for which $\sigma_s^{1500 \text{ K}} = 45 \text{ MPa}$.

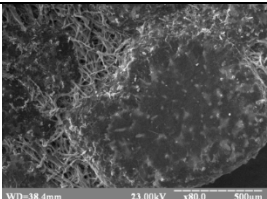
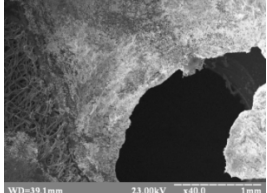
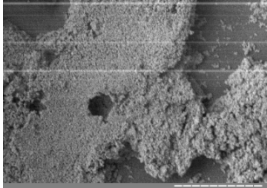
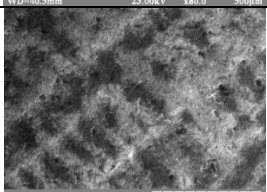
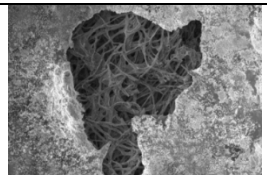
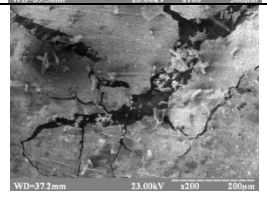
Thus, solving the problem of ensuring the quality of solder joining of elements in a single design requires the definition of rational solder conditions, the placement of ballasts for changing the conditions of absorption of radiant heat, as well as the scheme of loading the seams with clamping elements.

Microelectronic and photo-optical studies of the state of elements exposed to soldering in a vacuum are systematized and summarized in table 1. The composition of the material of the plates exposed to soldering, the tendency to form intermetallic inclusions and various defects of the structure

during heating, as well as high activity of the components to carbon, necessitated the complete abandonment of graphite-containing substrates and expanded stacks, since in this case, the processes of adhesion were actively manifested and there was no qualitative seam; the microelectronic investigation showed the presence of a graphitized layer, which reduces mechanical properties, mainly in the zone around the seam. Lowering the temperature to prevent curvatures deprived the ability to receive a molten solder in the contact zone of connecting elements (as a result of which the seam simply crumbled), and the temperature rise of more than 1750 K resulted in the combustion of samples on the stocks.

We also observed a characteristic of the alloy, manifested in involuntary start the exothermic reaction in some points of the surface, as a result of which it could be formed burnout of the material.

Table 1. Condition of elements and defects that occur when soldering

Research result	Soldering modes	Micro and macro photos	
Adhesion of the specimen before the substrate	$T=1300^{\circ}\text{C}$, $\tau=20\text{ min}$, $p=10^{-1}\text{ Pa}$		
Burnout of the part of material, fistula formation	$T=1380^{\circ}\text{C}$, $\tau=15\text{ min}$, $p=10^{-1}\text{ Pa}$		
Incomplete soldering with a fault under the action of a bending moment	$T=1250^{\circ}\text{C}$, $\tau=20\text{ min}$, $p=10^{-1}\text{ Pa}$		
Deformation of the finer part of the connection	$T=1380^{\circ}\text{C}$, $\tau=15\text{ min}$, $p=10^{-1}\text{ Pa}$		
The appearance of the fistula and the porosity of the seam	$T=1400^{\circ}\text{C}$, $\tau=15\text{ min}$, $p=10^{-1}\text{ Pa}$		
Cracking and fracture of a thinner plate	$T=1380^{\circ}\text{C}$, $\tau=20\text{ min}$, $p=10^{-1}\text{ Pa}$		

Use nickel powder without additives as solder led to the fact that the melt layer acquired a fibrous structure and did not provide a seam density. At the same time, the small amount of W in the solder precedes the occurrence of pores in the steam and the area around the seam.

At this stage, a number of unsatisfactory results were received which can be divided into the following groups:

- 1) Adhesion of the specimen before the substrate;
- 2) Combustion of the specimen when there is cobalt in the chamber;
- 3) Incomplete soldering with a fault under the action of a bending moment as a result of temperature deflection in the furnace from a cycle given by controller during asymmetrical loading of the chamber;
- 4) Burnout of the part of the specimen, fistula formation;
- 5) Deformation of the finer part of the connection due to the temperature act and asymmetry of the applied load;
- 6) Cracking and fracture of a thinner plate;
- 7) The appearance of fistulas (both in machining and during sintering) and the porosity of the seam.

As a result of optimization of the soldering process, it was possible to obtain a satisfactory qualitative connection of two plates with different thicknesses overlapped with an overlap of

7,2 mm. The area of the adhesive contact during measurements is 68 mm^2 , cracks and leakiness at the contact point are completely absent. The thickness of the soldered joint is 0,05-0,15 mm and is due to the initial spatial deviations of the blanks at the point of contact.

To check the accuracy of predictive calculations for a rational mode of soldering, soldering 4 plates of different thicknesses into a single structure was performed in accordance with fig. 3.

Microelectronic studies of the soldering place and mechanical tests have shown the following. On a plate of the largest (0,8 mm) thickness, when a load greater than 25 N was applied, one joint was destroyed. There was also a spreading of solder on the contact surfaces, which not only worsened the appearance of the joint but also changed the mechanical properties of the plate. This is especially dangerous both from the point of view of a slight increase in the mass of the system and from the point of view of the changes in modulus of elasticity and the relative elongation of the base material.

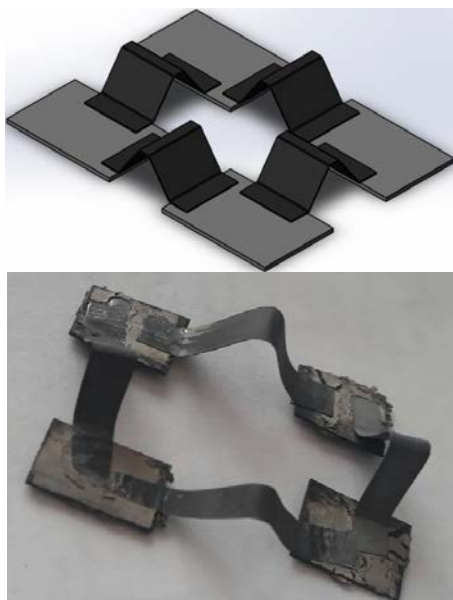


Fig. 3. Soldered structure from 4 plates of different thicknesses: 0,15 mm, 0,4 mm and 0,8 mm. The dimensions of the plates are 6×6 mm, the width of the connecting u-like tapes is 2,0 mm, the thickness of the tapes is 0,15 mm, the theoretical contact area is 7,0 mm²

Such a conclusion is made for the following reasons. The layer of solder that spreads on the surface has a porous structure, and in the case of alternating cyclic loads, it can cause cohesive damage of the material at the places of contact with the surface by the growth of microcracks oriented at angles to the contact surface.

We also proved the conclusion about the need for a correct geometric docking of the elements before welding, since the existing spatial deviations are not satisfactorily reflected in the strength of the joint.

Testing the strength of the resulting connection by force loading of the plates on the bursting machine showed that the destruction of the specimen occurred when the load reached 520 N, corresponding to the voltage at the intersection of the gap of 320±10 MPa, and the destruction itself was not on the welded seam, but in the zone of spreading solder on a plate, in a place in front of a soldered seam. The difference in the claimed strength limit of 991 MPa can be explained by the following reasons:

1) thin specimens exhibit somewhat different properties compared to the specimens in the form of rods, thick plates, etc.;

2) after welding by volumetric heating in the material, certain processes of intermetallide formation probably take place, which can reduce the ultimate strength, yield stress, elasticity and elongation of the material. To clarify these circumstances, more research is needed;

3) in the place of destruction, there are defects that can be stress concentrators, which reduces the resistance to fracture of the material.

In order to detect the effect of several soldering cycles on the mechanical properties of Ni-20Cr-6Al-1Ti-1Y2O3 alloy elements, we performed a duplication of heating with a thermal soldering cycle. It was established that after a 3-fold heating, thin plates of the experimental specimens began to be rapidly destroyed with the formation of end defects in the form of burns and fistulas.

Thus, since the soldering temperature of the elements with high-temperature solders is 1350-1375°C, it can be concluded that it is desirable to assemble the construction with the minimum number of operations (possibly one).

Consequently, as a result of our work, we were able to gradually test the technologies of obtaining the welded-soldered joints elements into a single system and prove the perspective of using Ni-20Cr-6Al-1Ti-1Y2O3 material for use in ultra-light thermal protection of reusable spacecraft with appropriate technological upgrading of the design, refining it to processability and adapting to the conditions of assembly into a single system.

3. CONCLUSION

As a result of the work, samples of permanent joints were obtained: a single plate, a model of a multiplanar system with u-shaped bridges; sample mock-up.

It has been established that a dense non-porous seam is obtained with the use of solders БИп36 (WPr36) and own solder with a content of W 8-9%, and the process of vacuum soldering should take place at a temperature of 1350°C for 15-20 minutes. The strength of the obtained compound is 390-420 MPa when the specimen is stretched by a tensile machine (with the appearance of tangential stresses). Surfaces for connection must be cleaned chemically and mechanically up to R_a 1,25-2,5 μm, non-flatness and deformation of the surfaces are not allowed (permissible deviation is 0,03 mm/100 mm of reference length).

The soldering of the heat-protective system is desirable to be carried out in a single setup in a vacuum chamber, while the control of the process should be carried out at the temperature in the soldering spot.

Promising is the approach of using heat shields and heat conductors, which at the same time serve as means for compressing the soldering zone to a value of 0,6-0,8 MPa.

4. REFERENCE

- [1] Metallic Thermal Protection System Requirements, Environments, and Integrated Concepts / John T. Dorsey, Carl C. Poteet, Kathryn E. Wurster et al. Journal of Spacecraft and Rockets. 41 (2) (2004) 162-172.
- [2] Improving Metallic Thermal Protection System Hypervelocity Impact Resistance Through Numerical Simulations / Carl C. Poteet, Max L. Blosser. Journal of Spacecraft and Rockets. 41 (2) (2004) 221-231.
- [3] Metallic Thermal-Protection-System Panel Flutter Study / Roger R. Chen, Max L. Blosser. Journal of Spacecraft and Rockets. 41 (2) (2004) 207-212.

IMPACT OF THE DECARBURIZATION LAYER ON THE CRACK PROPAGATION IN HIGH FREQUENCY WELDED JOINT

Prof. Dr. Maksuti Rr.

Faculty of Applied Sciences, University of Tetova, Republic of Macedonia

rrahimmaksuti@yahoo.com

Abstract: High-frequency electric resistance welding (HFERW) is one of the most common process for production of longitudinal welded carbon steel pipes, suitable for line pipes, casing, and tubing. In the edges joining line of hot rolled coils is formed decarburization layer which sometimes appeared negative impact on the microstructure and mechanical properties of the welded joint, so the aim of this paper is to investigate impact of this layer on the crack propagation in the pipes welded joint, obtained by high frequency electric resistance welding (HFERW). Crack propagation in the pipes welded joint monitored by macro and microscopic analysis as well as by the hardness testing, along and transverse through decarburization layer. Results of this investigation brings additional knowledge about impact of the decarburization layer on the crack propagation in the high frequency electric resistance welded joint.

Keywords: DECARBURIZATION LAYER, WELDED JOINT, CRACK PROPAGATION

1. Introduction

Welding is a complex process and the quality of a welded joint is a function of interaction of significant number of variables, together with the microstructural changes attendant upon welding. High frequency electric resistance (HFER) conduction welding (HFERW) process is one of the most extensively methods for production high quality longitudinal seam welded carbon steel pipes, suitable for line pipe, casing and tubing. In this process, hot rolled coils is gradually formed into round shape through roll-forming stands, (Fig. 1) and its edges are joined by a combination of localized high-frequency electric resistance heating and forge pressure [1, 2, 3]. Most of these pipes are produced according to API Standard [4] plus client supplementary requirements. Under this heat input condition and forge pressure it is possible to improve the welded joint quality and productivity of longitudinal seam welded carbon steel pipes.

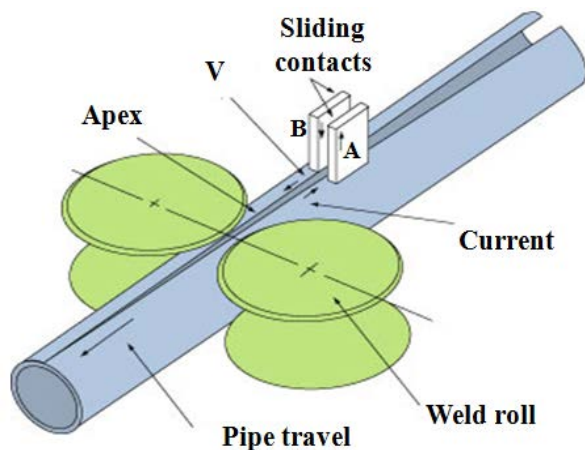


Fig.1 Schematic illustration of high-frequency conduction welding of steel pipes

The high-frequency current applied to the strip edges through sliding contacts, concentrated on the surface layer of the coils edges and due to the “skin” and “proximity” effects, generate joule heat and the hot “Vee” converge edges are forged together between the weld squeeze rolls, forming a forge type welded joint [5]. The HF welded joint is a true forge weld, in that no filler metal is added and, if done properly, no molten or oxidized metal is left on the bond line (BL). All of the molten thin layer and metal oxides and other inclusions are squeezed out of the welded joint, toward the outside and inside surfaces as the edges pass between the welding rolls (Fig. 2).

The removal of molten metal from the weld zone is beneficial because it eliminates the potentially harmful effects associated with cast structures, such as impact toughness, fracture toughness, etc.

The high frequency current follows a “Vee” shaped path down one edge of the “Vee” and up the other, from one sliding contact (A) to the other (B), completing electrical circuit, (Fig. 1).

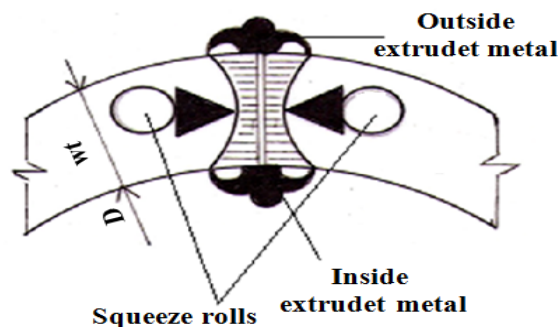


Fig. 2 High frequency forge type welded joint

From the metallurgical point of view, high frequency electric resistance conduction welding (HFERW) is characterized by extremely rapid heating and cooling over a very short period of time combined with forging pressure. The heat for welding, therefore, is developed in a small volume of metal along the surfaces to be joined. Thermal cycle (heating and cooling) combined with forging pressure are important metallurgical factors for welded joint integrity. As a result of these metallurgical factors some complex microstructure changes can occur.

The material extruded on the inside and outside weld surfaces, usually removed by mechanical cutting while still hot and forms a typical high frequency electric resistance welded joint with narrow bond line (BL) or fusion line (FL) and associated local heat affected zone (HAZ) is formed [5]. The high frequency electric resistance welded joint is subjected to local post weld heat treatment (LPWHT) in-line, the purpose of which is to eliminate zones of excessive hardness, because such zones could be susceptible to various forms of environmental cracking.

The normal high frequency electric resistance welded joint is shown in (Fig. 3). Note that the heat affected zone (HAZ) is shaped like an hourglass [5]. Fusion line (FL) or weld bond line (BL) is in the centre of the welded joint, perpendicular to the pipe wall thickness. The flow lines are symmetrical around the bond line (BL).

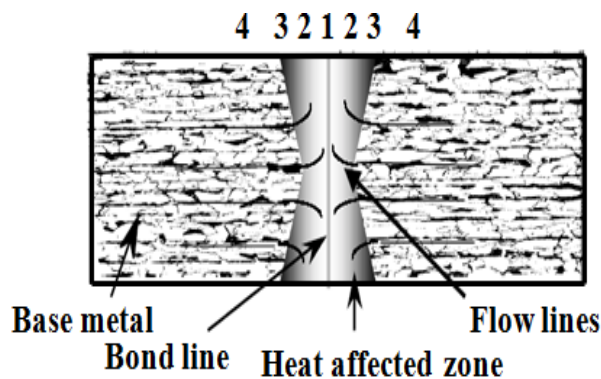


Fig. 3 High frequency electric resistance welded joint

The plastic deformation which is performed under the action pressure of the squeezing rolls caused metal flows of the hot rolled coils towards the outside and inside surfaces of the bond line (BL). This flow pattern consists of streaks and striations. The orientation of this pattern, with respect to the new surface, indicates the direction of metal flow lines (fibres), respectively flow angles during plastic deformation [6].

Forge weld area of high frequency electric resistance welding (HFERW) may be divided into four zones, (Fig. 3): 1-bond line (BL) or fusion line (FL), 2-heat affected zone (HAZ), 3-edge of the heat affected zone (EHAZ) and 4-base metal (BM). These different zones are normally defined by the peak temperature experienced at certain distance from the fusion line during welding. Each zone in the weld area is characterized by a unique microstructure and hence different mechanical properties [5]. These zones of the welded joint are quite narrow and it is difficult to investigate the behavior of specific location without interference from the adjacent zones with different properties.

The bond line (BL) is formed by the edges contact of hot rolled coils and its shape and sizes depend on the welding thermal cycle and forging pressure of the squeezing rolls, respectively on the intensity of deformation. In literature [6], the bond line (BL) is also known as the light area (LA). It is worth to mentioned that the bond line (BL) represents a zone where the composition of carbon is mostly smaller than the composition of the carbon in the base metal (BM), therefore, this zone is also called a decarburization zone (DZ) or decarburization layer (DL), fusion line (FL), melting zone (MZ), ferrite band (FB), etc. [7, 8, 9].

During welding, as a result of the high temperature, partially base metal (BM) melting occurs in butting (roughness) surfaces and thus begins the diffusion of the carbon atoms that goes towards the hottest part of the edges because that is most soluble in austenite and its interacts with the surrounding atmosphere, mainly with oxygen, carbon dioxide and water vapor, and forms the decarburization layer with a certain gradient of carbon composition in the opposite direction from the edges of the hot rolled coils. As a result of decarburization, the metal loses some of its strength and hardness and it may develop cracks which make it vulnerable to breaking. Unfortunately, the literature shows that decarburization of steel is a phenomenon slightly studied during these last decades.

There are different hypotheses about the formation of the decarburization layer (DL) during high frequency electric resistance welding (HFERW) and impact of this decarburization layer (DL) on the microstructure and mechanical properties of the welded joint [6].

According to [6], the decarburization layer (DL) presents a metallurgical defect, so the aim of this investigation is to explain the impact of this layer on the fracture behavior of the welded joint, respectively on the crack propagation in the welded joint, as the main stage before fracture.

2. Experimental procedure

2.1. Material

High-frequency electric resistance welding (HFERW) was conducted in manufacturing line (L-16 in), pipe mill Newco IMK-Ferizaj, Kosova. Pipes $\varnothing 114.3 \times 5.21 \text{ mm}$ were fabricated from high strength steel coils J55 according to API [4] standard, using 400 kHz Thermatool. The chemical composition and mechanical properties of hot rolled steel coils API Grade J55 [4], according to the manufacturer's Certificate are presented in Tab. 1, respectively 2.

Table 1: Chemical composition of used steel coils API Grade J55

Steel coils	Chemical composition [wt-%]							
	C	Mn	Si	P	S	Al	Nb	N
API Grade J55	0.141	1.113	0.229	0.014	0.008	0.047	0.017	0.0072

Table 2: Mechanical properties of used steel coils API Grade J55

Steel coils	Re	Rm	Re/Rm	A ₂ ”
	MPa			%
API Grade J55	453	557	0.81	32.5

2.2. Testing

With the purpose of fulfilling the aim of the investigation, samples are taken from the high frequency electric resistance welded pipes $\varnothing 114.3 \times 5.21 \text{ mm}$, (Fig. 4), for the following testing:

- flattening testing,
- metallographic analysis (macro and microscopic) of cracked samples after flattening testing,
- hardness testing (HV30/15).

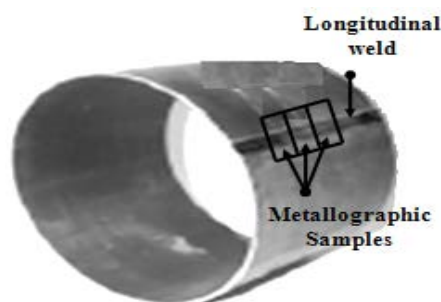


Fig. 4 Sketch illustrating the orientations of the samples used

The ring shape samples for flattening testing, after the edge preparation are subjected to compression force (F_c) in the hydraulic press, type DIHNAFORIN PS 2043, (Fig. 5), according to the schematic illustration (a) and (b).

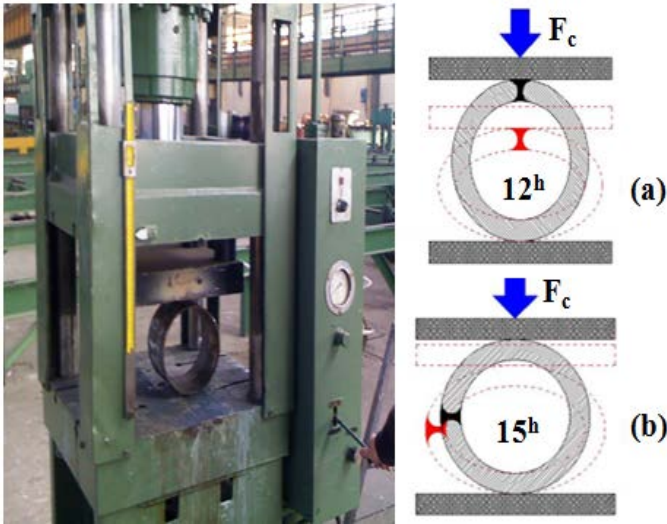


Fig. 5 Schematic illustration of flattening testing

From the pipe samples that have undergone the flattening tests, metallographic samples have been taken to observe the macrostructure and microstructure such as the propagation of cracks through the high frequency electric resistance welded joint.

Samples were prepared by standard metallographic techniques that includes grinding, polishing and etching with suitable etchant (3% Nital), within a few seconds.

The hardness testing (HV30/15) is conducted on the chosen samples across (a) and along (b) the bond line (BL). The hardness testing (HV30/15) is done on three directions A, B and C (Fig. 6), respectively in nine positions (1, 2, 3, 4, 5, 6, 7, 8, 9), across the bond line (BL) and on the D-D direction, respectively in five positions (1, 2, 3, 4, 5), along the bond line (BL), according to the scheme in (Fig. 6).

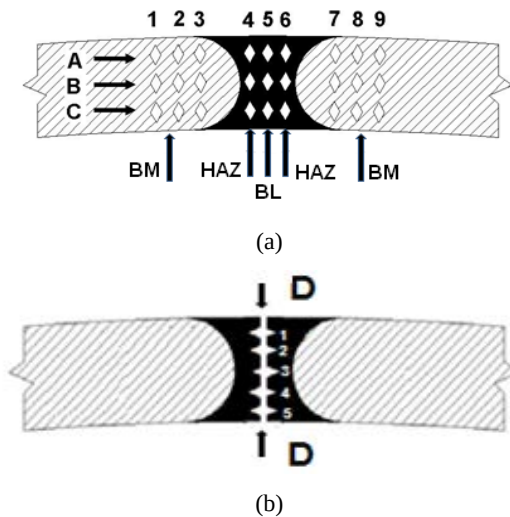


Fig. 6 Scheme of hardness testing (HV30/15) of the welded joint

3. Results and discussion

During flattening testing the welded joint from the outside undergoes a tension deformation, while on the inside part undergoes a compression deformation. When carrying out this testing in some samples are created cracks that lead to the fracture of samples. With this it is shown that the plasticity of the welded joint is weak, as a result of microstructure formed by the interaction of local heating and forging pressure of the squeezing rolls.

Since the purpose of this investigation is to review the impact of the decarburization layer (DL) on the crack propagation of the high

frequency electric resistance welded joint, samples with cracks are subjected to further investigations using metallographic macro and micro analysis.

During the flattening testing, respectively, during the deformation of samples in the hydraulic press, the behavior of the welded joint has been continuously observed during the action of compression force. The welded joint is positioned at 0° or as otherwise stated at 12° , (Fig. 5a) and at 90° or as otherwise stated 15° , (Fig. 5b), to the applied compression force (F_c), and the ring flattened to a specific height or until the appearance of the first cracks in the welded joint.

Metallographic samples after etching reveals constitutive parts of the welded joint (base metal-BM, heat affected zone-HAZ and decarburization layer-DL or bond line (BL). It can clearly reveal the presence of decarburization layer (DL), mostly vertically oriented through the pipe wall thickness or eventually little slanting related to the outside and inside of the pipe wall thickness, depending on the intensity and symmetry of the forging pressure of the squeezing rolls.

Through the macro metallographic analysis, (Fig. 7), it is clearly stated that the initiation of cracks occurs outside of the decarburization layer (DL) or bond line (BL), at the point (S-start) and the propagation of crack continue outside the decarburization layer (DL) and ends inside the material, at points (E1 and E2-end), which means that decarburization layer is not a potential causer for the initiation and propagation of cracks [10, 11].

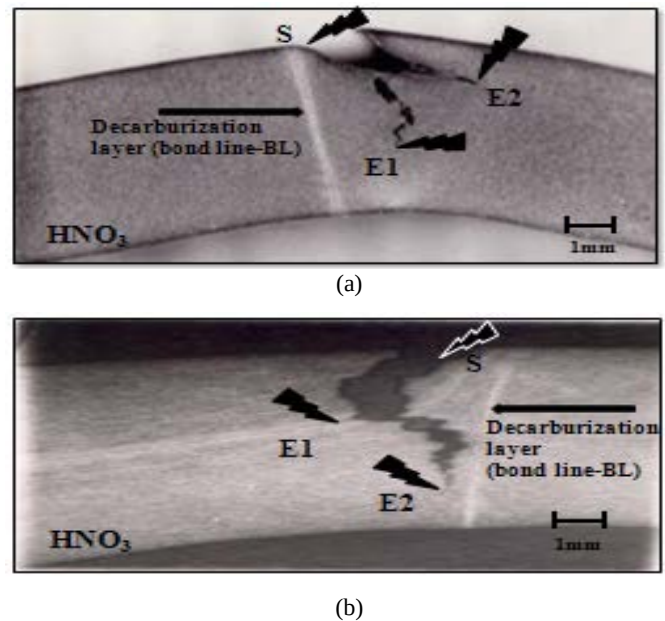
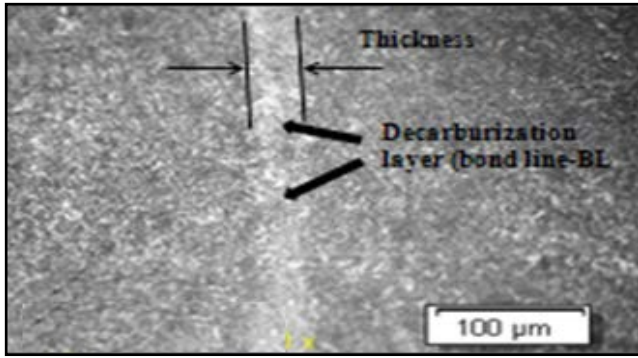


Fig. 7 Initiation and propagation of cracks in the welded joint

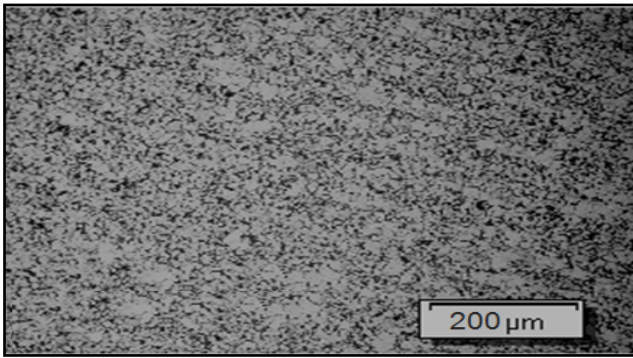
Propagation of cracks in both samples is in base metal (Fig. 7a) or in heat affected zone (Fig. 7b) and it is worth to mentionet that the end of the cracks in all investigatet samples is in base metal (BM) or in heated affected zone (HAZ), out of decarburization layer or bond line (BL).

Cracks initiated during flattening testing, propagate or grow in depth and length, but in all cases outside of the decarburization layer (DL) or bond line (BL), and it is clear to conclude that fracture of the welded joint will occur outside of decarburization layer (DL) or bond line (BL).

The micro metallographic microscopic analysis, (Fig. 8) reflects the decarburization layer (DL) or bond line (BL) which is perpendicular to the pipe wall thickness and is defined by certain uniform thickness within pipe wall thickness (Fig. 8a). This white area, microstructurally mainly is allotriomorphic or polygonal ferrite (Fig. 8b).



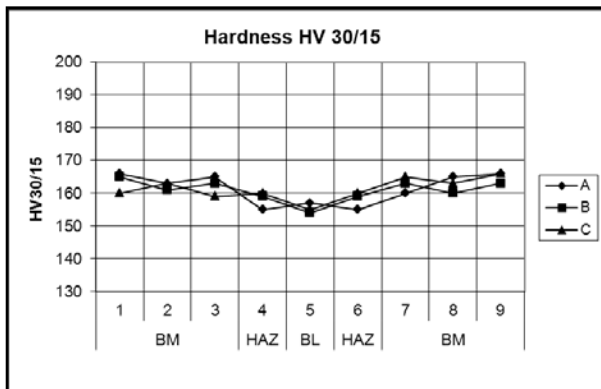
(a)



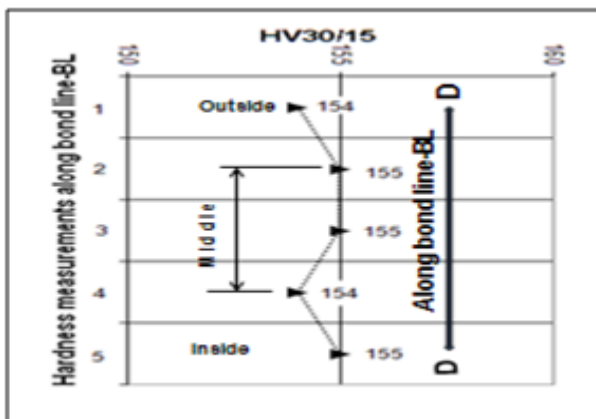
(b)

Fig. 8 Decarburization layer of the welded joint

By measuring the hardness (HV30/15) of the constitutive parts of the welded joint (BM, HAZ, DL/BL), is noticed that there is small difference between hardness of these constitutive parts of welded joint (Fig. 9).



(a)



(b)

Fig. 9 Hardness profiles (HV30/15) of the welded joint

4. Conclusion

Following conclusions can be drawn from the present investigation:

Decarburization layer (DL) or bond line (BL) during the production of high frequency electric resistance welding (HFERW) is due to simultaneous interaction between thermal cycle and forging pressure of the squeezing rolls.

Decarburization layer (DL) or (bond line (BL) has not indicated any significant negative impact on the fracture behavior of the high frequency electric resistance welded joint, other than symbolic reduction of hardness (HV30/15). Therefore, it cannot be said that there was any intolerant or serious metallurgical defect.

The initiation and propagation of cracks occurs outside of decarburization layer (DL) or bond line (BL) and that implies that this layer is not a potential cause of the initiation and propagation of cracks in the high frequency electric resistance welded joint as the main stage before fracture.

5. References

- [1] Choi J. H., Chang Y. S., Kim C. M., Oh J. S., and Kim Y. S., Penetrator Formation Mechanisms during High-Frequency Electric Resistance Welding, *Welding Journal*, 27s-31s, January 2004.
- [2] Kim D., Kim T., Park Y., W., Sung K., Kang M., Kim C., Lee C., and Rhee S., Estimation of Weld Quality in High-Frequency Electric Resistance Welding with Image Processing, *Welding Journal*, 71s-79s, March 2007.
- [3] Jeff P., Mike D., High Frequency Electric Resistance Welding-An Overview, *Practical Welding Today*, June 1, 2010.
- [4] API-American Petroleum Institute Specification for line pipe, Washington DC, July 2000.
- [5] Nicols R.K., The Metallurgical Effects of Weld Seam Heat Treating, *Thermatool Corp. Publication*, East Haven, CT, April 1998.
- [6] Zak B., Y., and Rys P., The origin of "Light Area" in upset welds of rolled carbon steel, *Welding Research Supplement* 5, 262s-279s, 1972.
- [7] Changchun Y., U., Metallographic examination evaluation criteria and control for ERW pipe production, *Tube International* 3/1996, 153-155.
- [8] Jack H. D., William E. W., *Principles of Joining Metallurgy*, Oregon Graduate Center, 1985.
- [9] Tetsuo K., Chiharu T., Kazuyuki H., Masao T., Shin N., Automatic Welding Control System for Electric Resistance Weld Tube Mill., *Transactions ISIJ*, Vol. 24, 1984, 847-856.
- [10] Maksud Rr., Mehmeti H., Oettel H., The Influence of the plastic deformation on the metal flow during high frequency electric resistance welding of longitudinally welded pipes, 3rd International Conference, Deformation Processing and Structure of Materials, Belgrade, Serbia, 20-22, September 2007.
- [11] Maksud Rr., Microstructural Changes in the Forge Weld Area During High Frequency Electric Resistance Welding, *International Journal for Science, Technics and Inovations for the Industry*, Year 10, Issue 5/2016, 23-26.

MODELING AND SIMULATION OF INDUSTRIAL PROCESSES

Christo Boyadjiev
Institute of Chemical Engineering, Bulgarian Academy of Sciences
chr.boyadjiev@gmail.com

Abstract: In the paper are presented the main theoretical techniques used for the modeling and simulation of industrial processes. The main focus is on the physical side of the theoretical techniques and their mathematical side is reduced to a reasonable minimum. Different theoretical approximations as thermodynamic and hydrodynamic levels are used.

KEYWORDS: MODELING, SIMULATION, THEORETICAL APPROXIMATION, THERMODYNAMIC LEVEL, HYDRODYNAMIC LEVEL, MECHANISM IDENTIFICATION, PARAMETERS IDENTIFICATION, STATISTICAL ANALYSIS.

1. Introduction

The modeling and simulation are a basic approach to quantifying processes and phenomena [1-3]. They have become realistic as a result of the development of computing and applied mathematics. In the industry, the modeling and simulation offer a quantitative description of the kinetics of processes and systems for the purposes of their optimal design or control. In the industrial systems, the process models of the individual devices are known in advance, and system models offer quantitative descriptions of the systems (process systems engineering).

In the industry, quantification of systems can also be used for various other tasks. For example, in periodically operating systems, the optimal schedules of the apparatuses (machines) for conducting different processes (operations) of different duration and different sequence to obtain different substances (machined details) can be determined. In these cases, the mass service theory offers models that allow for optimal solutions.

The fundamentals of the modeling and simulation, as a part of human knowledge and science, are related to the combination of intuition and logic. They are in different scales in the individual sciences [4, 5]. In the mathematics, logic dominates intuition, where intuition is the axiom (unconditional truth that is not proof able), and logic is the theorem (the logical consequences of the axiom). In the natural sciences (physics, chemistry, biology), the logic/intuition ratio is maintained, but axioms are usually conditional (principles, postulates, laws). This ratio goes back to the humanities and reaches the extreme in religion.

The modeling and simulation offer quantitative (mathematical) descriptions that have different degrees of detail. The lowest level is the thermodynamic (non-equilibrium thermodynamics) that examines the volume of the phase (gas, liquid, solid). The next level is the hydrodynamic, which examines the elementary phase volumes (mechanics of continua), which are much smaller than the phase volumes, but much larger than the intermolecular volumes, i.e. the molecules are indistinguishable. The highest level is the molecular (the kinetic theory of the ideal gas).

The modeling and simulation of industrial processes has a wide application, so the processes in the chemical industry and related biotechnologies and heating technologies, will be discussed. The major part of these processes is the transfer of mass and heat as a result of phase or phase boundary reactions. By reaction, will be understand the creation or disappearance of a particular substance (or amount of heat) as a result of a chemical reaction in the phase or on the phase boundary, interphase mass transfer, adsorption on the phase boundary or a liquid-vapor-liquid phase transition. These reactions result in varying concentrations and temperatures in the phases, i. e. to a deviation from the thermodynamic equilibrium and as a result of the mass transfer and heat transfer to restore the thermodynamic equilibrium. The models of the mass transfer and heat transfer are analogous and, therefore, the models of mass transfer in industrial processes will be presented.

2. Thermodynamic approximation

The reactions deviate the industrial systems from the thermodynamic equilibrium and the industrial processes for its recovery begin. The determining of the rate of these processes is a major problem in the industry, as it is the basis for their optimal design and control. This gives reason to use the thermodynamic laws of irreversible processes such as mathematical structures in the construction of the process models, described by extensive and

intense variables (in the case of merging of two identical systems, the extensive variables double their values, while the intensive variables retain their values).

The kinetics of the irreversible processes uses the mathematical structures, resulting from Onsanger's "linearity principle" [6]. According to him, the mean values of the derivatives at the time of the extensive variables depend linearly on the mean deviations of the conjugated intensive variables from their equilibrium states (values). This principle is valid in the vicinity of the equilibrium, and proportionality coefficients are kinetic (rate) constants.

According to the principle of linearity, the mass derivative at time

$J_0 = \frac{dm}{dt}$ [kg-mol.s⁻¹] depends linearly on the deviation from the

thermodynamic equilibrium ΔC [kg-mol.m⁻³] of the concentration in two phase volumes or in one phase and the phase boundary, i.e.

$$J_0 = k_0 \Delta C, \quad (1)$$

where k_0 [m³.s⁻¹] is a proportionality coefficient.

Consider a system that contains two identical volumes in one phase $V_1 = V_2 = V$ [m³]. The system contains a substance whose masses

m_i [kg-mol] and concentrations $C_i = \frac{m_i}{V_i}$ [kg-mol.m⁻³] are

different in two volumes, $i = 1, 2, \dots$. The system is not in

thermodynamic equilibrium. Let us assume for certainty

$C_1 - C_2 > 0$, $i = 1, 2$. As a result, the mass of the substance

starts to be transferred from volume V_1 to volume V_2 for to

achieve the equilibrium. According to the principle of linearity, the

mass transfer rate between the two volumes J_0 [kg-mol.s⁻¹] can be represented as:

$$J_0 = \frac{dm_1}{dt} = -\frac{dm_2}{dt} = k_0 (C_1 - C_2), \quad (2)$$

where k_0 [kg-mol⁻¹.m³.s⁻¹] is a proportionality coefficient. If we

replace masses with concentrations $m_i = V_i C_i$, $i = 1, 2$, the mass

transfer rate in one phase J [kg-mol.m⁻³.s⁻¹] between two points with different concentrations is:

$$J = \frac{dC_1}{dt} = -\frac{dC_2}{dt} = k (C_1 - C_2), \quad (3)$$

where k [s⁻¹] is a rate coefficient. This equation is capable of presenting the rate of interphase mass transfer in the case of adsorption or catalytic process, where C_1 is the concentration of the

substance in the gas phase, while C_2 is the concentration of the substance in the gaseous portion of the solid (capillaries of the adsorbent or catalyst) phase.

In the cases, where the volumes $V_1 = V_2 = V$ are in different phases (for example, 1 is a gas phase and 2 is a liquid phase), the

thermodynamic equilibrium law has the form $C_1 - \chi C_2 = 0$, i.e. this is the Henry's law and χ is the Henry's number. If $C_1 - \chi C_2 > 0$ the mass transfer is from phase 1 to phase 2 and the mass transfer rate between phases is:

$$J = k(C_1 - \chi C_2), \quad (4)$$

where k [s^{-1}] is the rate coefficient of the interphase mass transfer. On the surface between two phases, the thermodynamic equilibrium is immediately established, practically, i.e. $C_1^* - \chi C_2^* = 0$, where C_i^* , $i = 1, 2$, are the equilibrium concentrations on the phase boundary. Thus, the mass transfer rate can be expressed by mass transfer rate in two phases:

$$J = k_1(C_1 - C_1^*) = k_2(C_2^* - C_2), \quad (5)$$

where k_i , $i = 1, 2$ [s^{-1}] are mass transfer rate coefficients.

The Onsanger principle of linearity represents the thermodynamic approximation of the mathematical description of the kinetics of irreversible processes, but it does not show the way to reach equilibrium, i.e. the mechanism of the process and as a result the rate coefficient is not known. Obviously, this "thermodynamic level" does not allow a real quantitative description of the kinetics of irreversible processes in industry and the next level of detail of the description, the so-called "hydrodynamic level", should be used.

3. Hydrodynamic approximation

The processes in the chemical industry and related biotechnologies and heating technologies are realized in one-, two- and three-phase systems (gas-liquid-solid). They are a result from the reactions, i.e. processes of disappearance or creation of any substance. The reactions are associated with a particular phase and can be homogeneous (occurring in volume of the phase) or heterogeneous (occurring at the interface with another phase). Homogeneous reactions are usually chemical, while heterogeneous reactions may be chemical, catalytic and adsorption. Heterogeneous reaction is the interphase mass transfer too, where on the interphase boundary the substance disappears (created) in one phase and creates (disappears) in the other phase.

The volume reactions lead to different concentrations of the reagents in the phase volumes and as a result two mass transfer processes are realized – convective transfer (caused by the movement of the phases) and diffusion transfer (caused by the concentration gradients in the phases). The mass transfer models are a mass balance in the phases, where components are convective transfer, diffusion transfer and volume reactions (volume mass sources or sinks). The surface reactions participate as mass sources or sinks in the boundary conditions of the model equations. The models of this complex process are possible to be created on the basis of the mass transfer theory, whose models are created by the models of the hydrodynamics, diffusion and reaction kinetics. The mass transfer theory combines the chemistry, physics and mathematics and builds its logical structures on three main "axioms":

1. The postulate of Stokes for the linear relationship between the stress and deformation rate, which is the basis of the Newtonian fluid dynamics models;
2. The first law of Fick for the linear relationship between the mass flow and the concentration gradient, which is the basis of the linear theory of the mass transfer;
3. The first law of Fourier for the linear relationship between the heat flux and the temperature gradient, which is the basis of the linear theories of the heat transfer.

These are the laws of the impulse, mass and energy transfer.

In Boltzmann's kinetic theory of the ideal gas, these axioms are replaced by the "elastic shock" axiom (in a shock between two molecules the direction and the velocity of the movement change, but the sum of their kinetic energies is retained, i.e. there is no loss of kinetic energy) and the rate coefficients are theoretically

determined by the average velocity and the average free run of the molecules.

The contemporary mass transfer theory is based of diffusion boundary layer theory (Landau, Levich [7]). This approach substitutes (physically justified) elliptic partial differential equations with parabolic partial differential equations, which facilitates their mathematical solution and offers a mathematical description of physical processes with free (not predetermined) ends.

The diffusion boundary layer theory is developed in the cases of drops and bubbles (Levich, Krylov [8]), film flows (Levich, Krylov, Boyadjiev, Beshkov[9, 10]), non-linear mass transfer and hydrodynamic stability (Krylov, Boyadjiev, Babak [11, 12]).

3.1. Mass transfer theory

The complex industrial processes are a collection of elementary physical and chemical processes. For example, the chemical absorption in a packed bed column represents a physical absorption of a gas phase component in the liquid phase and a subsequent chemical reaction with a component of the liquid phase. The gas moves in the column like jets and bubbles, while the liquid moves in the form of drops, jets, and flowing films on the surface of the packed bed. As a result, the chemical absorption in a packed bed column is a combination of many elementary physical and chemical processes, as absorption in the systems gas-liquid drops, liquid-gas bubbles, gas-liquid film flow, etc. As an example will be considered the gas absorption in liquid film with free interface.

Let us consider absorption of a slightly soluble gas in a laminar liquid film [9, 10] in a coordinate system (x, y) , flowing over a

flat vertical interface $(y = 0)$. The hydrodynamic model has the form:

$$\begin{aligned} \nu \frac{\partial^2 u_x}{\partial y^2} + g = 0, \quad \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} = 0; \\ y = 0, \quad u_x = 0, \quad u_y = 0; \quad y = h_0, \quad \frac{\partial u_x}{\partial y} = 0 \end{aligned} \quad (6)$$

and the velocity distribution is:

$$u_x = \frac{g}{2\nu}(2h_0y - y^2), \quad u_y = 0. \quad (7)$$

If these conditions the convection-diffusion model has the form:

$$\begin{aligned} \frac{g}{2\nu}(2h_0y - y^2) \frac{\partial c}{\partial x} = D \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right), \\ x = 0, \quad c = c_0; \quad x \rightarrow \infty, \quad c = c^*; \\ y = 0, \quad \frac{\partial c}{\partial y} = 0; \quad y = h_0, \quad c = c^*, \end{aligned} \quad (8)$$

where the thermodynamically equilibrium exists at the film interface $(y = h_0)$ and c^* denotes the equilibrium concentration.

The solid interface $(y = 0)$ is impenetrable for the diffusing substance with inlet concentration $C_0 < C^*$ (absorption). A film of length l will be considered.

The diffusion boundary layer thickness δ [2] is:

$$\delta = \sqrt{\frac{Dl}{u^*}} = \frac{l}{\sqrt{Pe}}, \quad Pe = \frac{u^*l}{D}, \quad \frac{\delta}{l} = \frac{1}{\sqrt{Pe}}, \quad u^* = \frac{gh_0^2}{2\nu}, \quad \frac{\delta^2}{h_0^2} = Fo = \frac{Dl}{u^*h_0^2}, \quad (9)$$

where u^* , Pe , Fo , are the film interface velocity, the Peclet and Fourier numbers.

The diffusion boundary layer thickness δ is less than liquid film thickness h_0 that permits the diffusion boundary layer

approximation to be applied. As a result, the next generalized variables can be introduced:

$$x = lX, \quad y = h_0 - \delta Y, \quad c = c_0 + (c^* - c_0)C, \quad (10)$$

$$\text{where } 0 = \frac{h_0}{l} \leq 10^{-2}.$$

The introduction of (10) into (8) yields:

$$\begin{aligned} (1 + FoY^2) \frac{\partial C}{\partial X} &= \frac{Dl}{u^* \delta^2} \left(Pe^{-1} \frac{\partial^2 C}{\partial X^2} + \frac{\partial^2 C}{\partial Y^2} \right); \\ X = 0, \quad C = 0; \quad X \rightarrow \infty, \quad C = 1; \\ Y \rightarrow \infty, \quad C = 0; \quad Y = 0, \quad C = 1, \end{aligned} \quad (11)$$

where Fo is a small parameter:

$$\frac{\delta^2}{h_0^2} = Fo < 10^{-1}, \quad \frac{\delta^2}{l^2} = Pe^{-1} \leq 10^{-2}. \quad (12)$$

The problem (11) in the diffusion boundary layer approximation ($10^{-2} \geq Pe^{-1} = 0$) has the form: namely:

$$\begin{aligned} (1 + FoY^2) \frac{\partial C}{\partial X} &= \frac{\partial^2 C}{\partial Y^2}; \\ X = 0, \quad C = 0; \quad Y = 0, \quad C = 1; \quad Y \rightarrow \infty, \quad C = 0. \end{aligned} \quad (13)$$

The mass transfer rate (J) in the liquid film flow with a length l is the average value of the local mass flux through the face interphase ($y = h_0$). On the other hand this rate can be presented using the mass transfer coefficient k . As a result

$$J = \frac{D}{l} \int_0^l \left(\frac{\partial c}{\partial y} \right)_{y=h_0} dx = k(c^* - c_0). \quad (14)$$

In the generalized variables, from (14) the Sherwood number (Sh) is possible to be obtained:

$$Sh = \frac{kl}{D} = -\sqrt{Pe} \int_0^1 \left(\frac{\partial C}{\partial Y} \right)_{Y=0} dX, \quad (15)$$

where $C(X, Y)$ is the solution of (13) [9, 10] developed by a perturbation method [2]:

$$Sh = \sqrt{\frac{6Pe}{\pi}} \left(1 - \frac{Fo}{6} - \frac{19Fo^2}{120} \right). \quad (16)$$

The examined example shows the theoretical techniques, used for the modeling and simulation of the elementary processes in a complex industrial process. The presence of the models of all elementary processes in a complex industrial process does not give a practical opportunity to synthesize its model. The role of modeling and simulation of elementary processes is the theoretical explanation of a number of physical and chemical effects observed experimentally in industrial processes. An illustrative example in this respect is the nonlinear theory of the mass transfer.

3.2. Non-linear mass transfer theory

The theory of the diffusion boundary layer [2] is the basis of modern linear mass transfer theory, where the convection-diffusion equation in (8) is linear, i. e. the velocity does not depend on the concentration. In a number of cases, the experimental results for the mass transfer rate are higher than the predictions of the linear theory [11, 12]. This is due to nonlinear effects, where the mass transfer influences the hydrodynamics and the velocity begin to depend on concentrations. These non-linear effects are related to the induction of secondary flows at the interphase boundaries as a result of interphase mass transfer. Such effects are the effect of large concentration gradients [11], the effect of Marangoni and the effect of Stephan flow [12].

The large concentration gradients create an intensive diffusion flux that have a hydrodynamic character, and a secondary flow is induces, directed at the normal of the interphase boundary and results in an additional convective mass transfer.

The effect of Marangoni is a result of the gradient of the surface tension on the interphase surface, as a result of the surface gradient of the temperature or surface active agents concentration on the liquid-gas (liquid) interphase, and induces a tangential flow. As a result of the continuity of the flow, there appears to be a much lower flow in the direction of the normal of the interphase boundary and consequently an additional convective flow. Because of this, this effect is relatively weak and occurs in motionless or slow moving fluids.

The Stephan's flow is a result of a phase transition liquid-steam at the interphase surface when the volume of the liquid (steam) increases (decreases) a thousand times. As a result, there is a secondary flow, directed to the normal of the interphase boundary, and an additional convective mass transfer.

In the above three cases, an additional hydrodynamic effect appears very often because the secondary currents disturb the hydrodynamic stability of the flows and self-organizing dissipative structures occur, which further accelerate the mass transfer [9]. To these effects can be added the Benar instability [12] in the case of a positive vertical gradient of the density of gases or liquids resulting from concentration or temperature gradients.

The theory of mass transfer allows the construction of the process model if its physical mechanism is known. The model thus obtained allows for the identification of this mechanism, i.e. the determining of the significant physical effects and rejection of the insignificant, using the generalized analysis method [2].

4. Physical mechanism identification

The qualitative analysis of the models permits to be made the physical mechanism identification, using generalized variables [2]. They are dimensionless variables, whereas as the characteristic (inherent) scales are used the maximal or average values of the variables. The introduction of the generalized variables leads to dimensionless model. As a result the unity is the order of magnitude of all functions and their derivatives in the model, i.e. the effects of the physical and chemical phenomena (the contribution of the terms in the model), are determined by the orders of magnitude of the dimensionless parameters in the model. If all model equations are divided by the dimensionless parameter, which has the maximal order of magnitude, all terms in the model equations will be classified in three parts:

1. The parameter is unity or its order of magnitude is unity, i.e. this mathematical operator represents a main physical effect;
2. The parameter's order of magnitude is 10^{-1} , i.e. this mathematical operator represents a small physical effect;
3. The parameter's order of magnitude is $\leq 10^{-2}$, i.e. this mathematical operator represents a very small (negligible) physical effect and has to be neglected, because it is not possible to be measured experimentally.

After the physical mechanism identification the model contains a minimum number of parameters which must be determined experimentally.

5. Parameters identification

In general case, the identification of the parameters in the model is made by the minimization of the least squares function by the inverse identification problem solution [1-3]. The least squares function represents the sum of the squares of the differences between the calculated and the experimental values of the functions in the model and its minimum must be obtained with respect to the parameters in the model. This inverse identification problem is very often incorrect and needs special methods for the solutions [2].

6. Statistical analysis of the model adequacy

The stochastic nature of the errors during the experimental data determination leads to subsequent errors of the model parameters. The model is adequate if the variance of the statistical error of the model does not exceed the variance of the statistical error of the experimental data, i. e. the accuracy of the functions calculation by the model is not less than the accuracy of the function experimental measurement [2, 3].

7. Processes simulation

The process simulation uses the most common numerical methods of applied mathematics to solve model equations. For this purpose, commercial software is usually used. In many cases, however, it is necessary to introduce this software into specialized algorithms [2, 13].

8. Modeling of industrial mass transfer processes in column apparatuses

The diffusion boundary theory is not applicable for the modeling of chemical, absorption, adsorption and catalytic processes in column apparatuses, where the velocity distributions and interphase boundaries are unknown.

The use of the physical approximations of the mechanics of continua for the interphase mass transfer process modeling in industrial column apparatuses is possible if the mass appearance (disappearance) of the reagents on the interphase surfaces of the elementary physical volumes (as a result of the heterogeneous reactions) are replaced by the mass appearance (disappearance) of the reagents in the same elementary physical volumes (as a result of the equivalent homogenous reactions), i.e. the surface mass sources (sinks), caused by absorption, adsorption or catalytic reactions must be replaced with equivalent volume mass sources (sinks). The solution of this problem is related with the creation of new type of convection-diffusion and average-concentration models [13].

The convection-diffusion models permit the qualitative analysis of the processes only, because the velocity distribution in the column is unknown. On this base is possible to be obtained the role of the different physical effect in the process and to reject those processes, whose relative influence is less than 1%, i.e. to be made process mechanism identification.

The average-concentration models are obtained from the convection-diffusion models, where average velocities and concentrations are introduced. The velocity distributions are introduced by the parameters in the model, which must to be determined experimentally.

Conclusions

The theoretical foundations of modeling and simulation of the industrial processes are presented. The first step is the formulation

of the physical mechanism of the industrial process and the construction of a mathematical structure, containing the mathematical operators that quantitatively describe the individual physical effects in this mechanism. The introduction of generalized (dimensionless) variables through characteristic scales permits to be made a quality analysis of the industrial processes. The obtaining of the experimental data and using it to calculate the model parameters by solving a inverse identification problem leads to the final form of the mathematical model. The statistical analysis of the model adequacy leads to the practical applicability of the mathematical model. The presented results are published in 8 monographies (www.iche.bas.bg/Books_BG.htm).

References

1. Хр. Бояджиев, Основи на моделирането и симулирането в инженерната химия и химичната технология, ИИХ-БАН, София, 1993. (Fundamentals of modeling and simulation in chemical engineering and chemical technology - Bulgarian).
2. Chr. Boyadjiev, Theoretical Chemical Engineering. Modeling and simulation, Springer-Verlag, Berlin Heidelberg, 2010.
3. Хр. Бояджиев, Основи на моделирането и симулирането в химичната промишленост, Изд. БАН „Проф. Марин Дринов“, София, 2017. (Fundamentals of modeling and simulation in chemical industry - Bulgarian).
4. Е. Л. Фейнберг, Две культуры. Интуиция и логика в искусстве и науке, БЕК 2, Фрязино, 2004, 286 сс. (Logic and intuition in art and science - Russian).
5. Chr. Boyadjiev, Some Thoughts on Logic and Intuition in Science and Chemical Engineering, Open Access Library Journal, 1, №6, 1-5, 2014.
6. Keizer J., Statistical Thermodynamics of Nonequilibrium Processes, Springer-Verlag, New York, 1987.
7. L. D. Landau, E. M. Lifshitz, Fluid Mechanics, Pergamon, Oxford, 1989.
8. V. G. Levich, Physicochemical Hydrodynamics, Prentice Hall, New York, 1962.
9. Chr. Boyadjiev, V. Beschkov, Mass Transfer in Liquid Film Flows, Publ. House Bulg. Acad. Sci., Sofia, 1984.
10. Хр. Бояджиев, В. Бешков, Массоперенос в движущихся пленках жидкости. Москва, Изд. „Мир“, 1988. (Mass Transfer in Liquid Film Flows - Russian).
11. В. С. Крылов, Хр. Бояджиев, Нелинейный массоперенос. Новосибирск, Изд. Институт теплофизики СО РАН, 1996. (Non-Linear Mass Transfer - Russian).
12. Chr. B. Boyadjiev, V. N. Babak, Non-Linear Mass Transfer and Hydrodynamic Stability, New York, ELSEVIER, 2000.
13. Chr. Boyadjiev, M. Doichinova, B. Boyadjiev, P. Popova-Krumova, Modeling of Column Apparatus Processes, Springer-Verlag, Berlin Heidelberg, 2016.

SIMULATION OF THE PROCESSES OF ENCODING AND DECODING WITH LINEAR BLOCK CODES DETECTING AND CORRECTING ERRORS

Assist. Prof. M.Sc. Borodzhieva A. PhD.¹, M.Sc. Aliev Y.², Assoc. Prof. M.Sc. Ivanova G. PhD²
Faculty of Electrical Engineering, Electronics and Automation – University of Ruse “Angel Kanchev”,
Bulgaria, Department of Telecommunications¹, Department of Computer Systems and Technologies²
aborodzhieva@uni-ruse.bg

Abstract: In coding theory, a linear code is an error-correcting code for which any linear combination of codewords is also a codeword. Linear codes are traditionally divided into block codes and convolutional codes. Linear codes allow more efficient encoding and decoding algorithms than other codes using the syndrome decoding. Linear codes are applied in methods for transmitting symbols on a communication channel so that, if errors occur in the communications, some errors can be corrected or detected by the recipient of a message block. The codewords in a linear block code are blocks of symbols that are encoded using more symbols than the original value to be sent. A (6, 3) linear block code example and its decoder implementation using Logisim, an educational tool for designing and simulating digital logic circuits, are given in the paper. The processes of encoding and decoding when detecting and correcting errors using this (6, 3) linear block code are illustrated. The material presented in the paper is used in the educational process in the University of Ruse.

Keywords: MODELING AND SIMULATION, LINEAR BLOCK CODES, LOGISIM, ACTIVE LEARNING METHODS

1. Introduction

Channel coding refers to the class of signal transformations designed to improve communications performance by enabling the transmitted signals to better withstand the effects of various channel impairments, such as noise, interference, and fading. These signal-processing techniques can be thought of as vehicles for accomplishing desirable system trade-offs (e.g., error-performance versus bandwidth, power versus bandwidth). The use of large-scale integrated circuits and high-speed digital signal processing techniques have made it possible to provide as much as 10 dB performance improvement through these methods, at much less cost than through the use of most other methods such as higher power transmitters or larger antennas [1, 2].

2. Linear block codes

Linear block codes are a class of parity-check codes described by the (n, k) notation. The encoder transforms a block of k message digits (a message vector) into a longer block of n codeword digits (a code vector) constructed from a given alphabet of elements. When the alphabet consists of two elements (0 and 1), the code is a binary code comprising binary digits (bits) [1].

The k -bit messages form 2^k distinct message sequences, referred to as k -tuples (sequences of k bits). The n -bit blocks form 2^n distinct sequences, referred to as n -tuples. The encoding process assigns one of the 2^n n -tuples to each of the 2^k message k -tuples. A block code represents a one-to-one assignment, whereby the 2^k message k -tuples are uniquely mapped into a new set of 2^k codeword n -tuples; the mapping can be accomplished via a look-up table. For linear codes, the mapping transformation is linear [1].

The set of all binary n -tuples, V_n , is called a vector space over the binary field of two elements (0 and 1). The binary field has two operations, addition and multiplication, such that the results of all operations are in the same set of two elements. The arithmetic operations of addition and multiplication are defined by the conventions of the algebraic field. For example, in a binary field, the rules of addition and multiplication are as follows: 1) $0 \oplus 0 = 0$, $0 \oplus 1 = 1 \oplus 0 = 1$, $1 \oplus 1 = 0$; 2) $0 \cdot 0 = 0$, $0 \cdot 1 = 1 \cdot 0 = 0$, $1 \cdot 1 = 1$. The addition operation, designated with the symbol $\oplus$, is the modulo-2 operation. The summation of binary n -tuples always entails modulo-2 addition.

A subset S of the vector space V_n is called a subspace if the following two conditions are met: 1) The all-zeros vector is in S . 2) The sum of any two vectors in S is also in S (known as the closure property). These properties are fundamental for the

algebraic characterization of linear block codes. Let V_i and V_j be two codewords (or code vectors) in an (n, k) binary block code. The code is said to be linear if, and only if $V_i \oplus V_j$ is also a code vector. A linear block code, then, is one in which vectors outside the subspace cannot be created by the addition of legitimate codewords (members of the subspace). For example, the vector space V_4 consists of the following $2^4 =$ sixteen 4-tuples: 0000, 0001, 0010, 0011, 0100, 0101, 0110, 0111, 1000, 1001, 1010, 1011, 1100, 1101, 1110, 1111. An example of a subset of V_4 that forms a subspace is: 0000, 0101, 1010, 1111. It seems that the addition of any two vectors in the subspace can only yield one of the other members of the subspace. A set of 2^k n -tuples is called a linear block code if, and only if, it is a subspace of the vector space V_n of all n -tuples. Fig. 1 illustrates the structure of linear block codes [1].

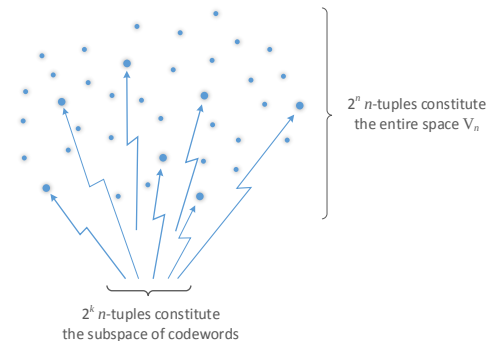


Fig. 1. Linear block-code structure [1]

The vector space V_n consists of 2^n n -tuples. Within this vector space there exists a subset of 2^k n -tuples forming a subspace. These 2^k vectors (points), shown “sprinkled” among the more numerous 2^n points, represent the legitimate (allowable) codewords. A message is encoded into one of the 2^k allowable code vectors and then transmitted. Because of noise in the channel, a corrupted version of the codeword (one of the other 2^n vectors in the n -tuple space) may be received. If the corrupted vector is not too distant from the valid codeword, the decoder can decode the message correctly. The basic goals in choosing a particular code can be stated in the context of Fig. 1 as follows: 1) for coding efficiency packing the V_n space with as many codewords as possible, to expend a small amount of redundancy (excess bandwidth); 2) the codewords must be as far apart from one another as possible, so that even if the vectors are corrupted during transmission, they may still be correctly decoded, with a high probability [1].

3. A (6, 3) linear block code example

The following coding assignment describing a (6, 3) code is examined. There are $2^k = 2^3 = 8$ message vectors, and therefore eight codewords. There are $2^n = 2^6 = 64$ 6-tuples in the V_6 vector space. It seems that the eight codewords in Table 1 form a subspace of V_6 (the all-zeros vector is present, and the sum of any two codewords yields another codeword member of the subspace). Therefore, these codewords represent a *linear block code*. A unique assignment for a particular (n, k) code does not exist; however, there is no complete freedom of choice.

Table 1. Assignment of codewords to messages

Message vector	Codeword
000	000000
100	110100
010	011010
110	101110
001	101001
101	011101
011	110011
111	000111

If k is large, a *table look-up* implementation of the encoder becomes prohibitive. For a (127, 92) code there are 2^{92} or approximately 5×10^{27} code vectors. The size of the memory necessary to contain such a large number of codewords is large, but it is possible to reduce the complexity by generating the required codewords as needed, instead of storing them [1].

Since a set of codewords that forms a linear block code is a k -dimensional subspace of the n -dimensional binary vector space ($k < n$), it is always possible to find a set of n -tuples, fewer than 2^k , that can generate all the 2^k codewords of the subspace. Generating the set of vectors is said to *span* the subspace. The smallest *linearly independent* set that spans the subspace is called a *basis* of the subspace, and the number of vectors in this basis set is the dimension of the subspace. Any basis set of k linearly independent n -tuples $\mathbf{V}_1, \mathbf{V}_2, \dots, \mathbf{V}_k$ can be used to generate the required linear block code vectors, since each code vector is a linear combination of $\mathbf{V}_1, \mathbf{V}_2, \dots, \mathbf{V}_k$. Each of the set of 2^k codewords $\{\mathbf{U}\}$ can be described by $\mathbf{U} = m_1\mathbf{V}_1 + m_2\mathbf{V}_2 + \dots + m_k\mathbf{V}_k$, where $m_i = (0 \text{ or } 1)$ are the message bits and $i = 1, \dots, k$. In general, the generator matrix is defined by the following $k \times n$ array [1]:

$$(1) \quad \mathbf{G} = \begin{bmatrix} \mathbf{V}_1 \\ \mathbf{V}_2 \\ \vdots \\ \mathbf{V}_k \end{bmatrix} = \begin{bmatrix} v_{11} & v_{12} & \dots & v_{1n} \\ v_{21} & v_{22} & \dots & v_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ v_{k1} & v_{k2} & \dots & v_{kn} \end{bmatrix}.$$

Code vectors are usually designated as row vectors. Thus, the message $\mathbf{m}$, a sequence of k message bits, is shown below as a row vector ($1 \times k$ matrix) $\mathbf{m} = m_1, m_2, \dots, m_k$.

The generation of the codeword $\mathbf{U}$ is written in matrix notation as $\mathbf{U} = \mathbf{m}\mathbf{G}$, where the matrix multiplication $\mathbf{C} = \mathbf{A}\mathbf{B}$ is performed in the usual way by using the rule $c_{ij} = \sum_k a_{ik}b_{kj}$, $i = 1, \dots, l$, $j = 1, \dots, m$, where $\mathbf{A}$ is an $l \times n$ matrix, $\mathbf{B}$ is an $n \times m$ matrix, and the result $\mathbf{C}$ is an $l \times m$ matrix. For the example in Table 1, the generator matrix is:

$$(2) \quad \mathbf{G} = \begin{bmatrix} \mathbf{V}_1 \\ \mathbf{V}_2 \\ \mathbf{V}_3 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 \end{bmatrix},$$

where $\mathbf{V}_1$, $\mathbf{V}_2$, and $\mathbf{V}_3$ are three *linearly independent* vectors (a subset of the eight code vectors) that can generate all the code vectors. The sum of any two generating vectors does not yield any of the other generating vectors. Generating the codeword $\mathbf{U}_4$ for the fourth message vector 110 in Table 1, using the generator matrix in Equation (2) is as follows:

$$\begin{aligned} \mathbf{U}_4 &= \begin{bmatrix} 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{V}_1 \\ \mathbf{V}_2 \\ \mathbf{V}_3 \end{bmatrix} = 1 \cdot \mathbf{V}_1 + 1 \cdot \mathbf{V}_2 + 0 \cdot \mathbf{V}_3 = \\ (3) \quad &= \begin{bmatrix} 1 & 1 & 0 & 1 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 1 & 1 & 0 & 1 & 0 \end{bmatrix} + \\ &+ \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 1 & 1 & 1 & 0 \end{bmatrix} \end{aligned}$$

The code vector corresponding to a message vector is a linear combination of the rows of $\mathbf{G}$. Since the code is totally defined by $\mathbf{G}$, the encoder needs only store k rows of $\mathbf{G}$ instead of the total 2^k vectors of the code. For this example, the generator matrix of size 3×6 in Equation (2) replaces the original codeword array of size 8×6 in Table 1, representing a reduction in system complexity [1].

A systematic (n, k) linear block code is a mapping from a k -dimensional message vector to an n -dimensional codeword in such a way that a part of the sequence generated coincides with the k message bits. The remaining $(n - k)$ bits are the parity bits. A systematic linear block code has a generator matrix of the form [1]:

$$(4) \quad \mathbf{G} = [\mathbf{P} \mid \mathbf{I}_k] = \begin{bmatrix} p_{11} & p_{12} & \dots & p_{1,(n-k)} & 1 & 0 & \dots & 0 \\ p_{21} & p_{22} & \dots & p_{2,(n-k)} & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ p_{k1} & p_{k2} & \dots & p_{k,(n-k)} & 0 & 0 & \dots & 1 \end{bmatrix},$$

where $\mathbf{P}$ is the parity array portion of the generator matrix, $p_{ij} = (0 \text{ or } 1)$, and $\mathbf{I}_k$ is the $k \times k$ identity matrix. With this systematic generator, the encoding complexity is further reduced since it is not necessary to store the identity matrix portion of the array. Each codeword is expressed as [1]:

$$\begin{aligned} [u_1, u_2, \dots, u_n] &= [m_1, m_2, \dots, m_k] \times \\ (5) \quad &\begin{bmatrix} p_{11} & p_{12} & \dots & p_{1,(n-k)} & 1 & 0 & \dots & 0 \\ p_{21} & p_{22} & \dots & p_{2,(n-k)} & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ p_{k1} & p_{k2} & \dots & p_{k,(n-k)} & 0 & 0 & \dots & 1 \end{bmatrix}, \end{aligned}$$

where $u_i = m_1p_{1i} + m_2p_{2i} + \dots + m_kp_{ki}$ for $i = 1, \dots, (n - k)$ and $u_i = m_{i-n+k}$ for $i = (n - k + 1), \dots, n$.

Given the message k -tuple $\mathbf{m} = m_1, m_2, \dots, m_k$ and the general code vector n -tuple $\mathbf{U} = u_1, u_2, \dots, u_n$, the systematic code vector can be expressed as $\mathbf{U} = \underbrace{p_1, p_2, \dots, p_{n-k}}_{\text{parity bits}}, \underbrace{m_1, m_2, \dots, m_k}_{\text{message bits}}$, where:

$$\begin{aligned} p_1 &= m_1p_{11} + m_2p_{21} + \dots + m_kp_{k1}, \\ (6) \quad p_2 &= m_1p_{12} + m_2p_{22} + \dots + m_kp_{k2}, \dots, \\ p_{n-k} &= m_1p_{1,(n-k)} + m_2p_{2,(n-k)} + \dots + m_kp_{k,(n-k)}. \end{aligned}$$

Sometimes systematic codewords are written in such a way that the message bits occupy the left-hand part of the codeword and the parity bits occupy the right-hand part. This reordering has no effect on the error detection or error correction properties of the code, and will not be considered further.

For the (6, 3) code example (Table 1), the codewords are described as follows:

$$(7) \quad \mathbf{U} = [m_1, m_2, m_3] \begin{bmatrix} 1 & 1 & 0 & | & 1 & 0 & 0 \\ 0 & 1 & 1 & | & 0 & 1 & 0 \\ 1 & 0 & 1 & | & 0 & 0 & 1 \end{bmatrix},$$

$$(8) \quad \mathbf{U} = \underbrace{m_1 + m_3}_{u_1}, \underbrace{m_1 + m_2}_{u_2}, \underbrace{m_2 + m_3}_{u_3}, \underbrace{m_1}_{u_4}, \underbrace{m_2}_{u_5}, \underbrace{m_3}_{u_6}.$$

Equation (8) provides some insight into the structure of linear block codes. The redundant digits are produced in a variety of ways. The first parity bit is the sum of the first and third message bits; the second parity bit is the sum of the first and second message bits; and the third parity bit is the sum of the second and third message bits. Such structure, compared with single-parity checks or simple digit-repeat procedures, may provide greater ability to detect and correct errors.

A matrix $\mathbf{H}$, called the *parity-check matrix*, enables to decode the received vectors. For each $(k \times n)$ generator matrix $\mathbf{G}$, there exists an $(n-k) \times k$ matrix $\mathbf{H}$, such that the rows of $\mathbf{G}$ are orthogonal to the rows of $\mathbf{H}$, i.e. $\mathbf{GH}^T = \mathbf{0}$, where $\mathbf{H}^T$ is the *transpose* of $\mathbf{H}$, and $\mathbf{0}$ is a $k \times (n-k)$ all-zeros matrix. To fulfill the orthogonality requirements for a systematic code, the components of the $\mathbf{H}$ matrix and the $\mathbf{H}^T$ matrix are written as [1]:

$$(9) \quad \mathbf{H} = [\mathbf{I}_{n-k} \mid \mathbf{P}^T],$$

$$(10) \quad \mathbf{H}^T = \begin{bmatrix} \mathbf{I}_{n-k} \\ \mathbf{P} \end{bmatrix} = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 \\ p_{11} & p_{12} & \dots & p_{1,(n-k)} \\ p_{21} & p_{22} & \dots & p_{2,(n-k)} \\ \vdots & \vdots & \ddots & \vdots \\ p_{k1} & p_{k2} & \dots & p_{k,(n-k)} \end{bmatrix}$$

It seems that the product $\mathbf{UH}^T$ of each codeword $\mathbf{U}$, generated by $\mathbf{G}$ and the matrix, yields

$$(11) \quad \mathbf{UH}^T = [p_1 + p_1, p_2 + p_2, \dots, p_{n-k} + p_{n-k}] = \mathbf{0},$$

where $p_1, p_2, \dots, p_{n-k}$ are the parity bits. Once the *parity-check matrix* $\mathbf{H}$ is constructed to fulfill the orthogonality requirements, it can be used to test whether a received vector is a valid member of the codeword set. $\mathbf{U}$ is a codeword generated by matrix $\mathbf{G}$ if, and only if $\mathbf{UH}^T = \mathbf{0}$.

Let $\mathbf{r} = r_1, r_2, \dots, r_n$ be a received vector (one of 2^n n -tuples) resulting from the transmission of $\mathbf{U} = u_1, u_2, \dots, u_n$ (one of 2^k n -tuples). Therefore $\mathbf{r}$ can be describe as $\mathbf{r} = \mathbf{U} + \mathbf{e}$, where $\mathbf{e} = e_1, e_2, \dots, e_n$ is an error vector or error pattern introduced by the channel. There are a total of $2^n - 1$ potential non-zero error patterns in the space of 2^n n -tuples. The *syndrome* of $\mathbf{r}$ is defined as

$$(12) \quad \mathbf{S} = \mathbf{rH}^T.$$

The syndrome is the result of a parity check performed on $\mathbf{r}$ to determine whether $\mathbf{r}$ is a valid member of the codeword set. If $\mathbf{r}$ is a member, the syndrome $\mathbf{S}$ has a value $\mathbf{0}$. If $\mathbf{r}$ contains detectable errors, the syndrome has some nonzero value. If $\mathbf{r}$ contains correctable errors, the syndrome has some nonzero value that can earmark the particular error pattern. The syndrome of $\mathbf{r}$ will be:

$$(13) \quad \mathbf{S} = (\mathbf{U} + \mathbf{e})\mathbf{H}^T = \mathbf{UH}^T + \mathbf{eH}^T.$$

However, $\mathbf{UH}^T = \mathbf{0}$ for all members of the codeword set. Therefore,

$$(14) \quad \mathbf{S} = \mathbf{eH}^T.$$

It is evident that the syndrome test, whether performed on either a corrupted code vector or on the error pattern that caused it, yields the same syndrome. An important property of linear block codes, fundamental to the decoding process, is that the mapping between correctable error patterns and syndromes is one to one.

It is interesting to note the following two required properties of the parity-check matrix: 1) No column of $\mathbf{H}$ can be all zeros, or else an error in the corresponding code-word position would not affect on the syndrome and would be undetectable. 2) All columns of $\mathbf{H}$ must be unique. If two columns of $\mathbf{H}$ were identical, errors in these two corresponding codeword positions would be indistinguishable.

Suppose that codeword $\mathbf{U} = 101110$ is transmitted and the vector $\mathbf{r} = 001110$ is received, i.e. the leftmost bit is received in error. The syndrome vector value $\mathbf{S} = \mathbf{rH}^T$ is found below and it is verified that it is equal to $\mathbf{eH}^T$. The syndrome of the corrupted code vector and the syndrome of the error pattern will be [1]:

$$(15) \quad \mathbf{S} = \mathbf{rH}^T = \begin{bmatrix} 0 & 0 & 1 & 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix}$$

$$(16) \quad \mathbf{S} = \mathbf{eH}^T = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \mathbf{H}^T = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix}$$

A single error is detected and it is shown that the syndrome test performed on either the corrupted codeword, or on the error pattern that caused it, yields the same syndrome. It means that the error not only can be detected, but since there is a one-to-one correspondence between correctable error patterns and syndromes, such error patterns can be corrected. Let arrange the 2^n n -tuples that represent possible received vectors in an array, called the *standard array*, such that the first row contains all the codewords, starting with the all-zeros codeword, and the first column contains all the correctable error patterns. From the basic properties of linear codes it is known that the all-zeros vector must be a member of the codeword set. Each row, called a *coset*, consists of an error pattern in the first column, called the *coset leader*, followed by the codewords corrupted by that error pattern. The standard array format for an (n, k) code is as follows:

$$(17) \quad \begin{array}{cccccc} \mathbf{U}_1 & \mathbf{U}_2 & \dots & \mathbf{U}_i & \dots & \mathbf{U}_{2^k} \\ \mathbf{e}_2 & \mathbf{U}_2 + \mathbf{e}_2 & \dots & \mathbf{U}_i + \mathbf{e}_2 & \dots & \mathbf{U}_{2^k} + \mathbf{e}_2 \\ \mathbf{e}_3 & \mathbf{U}_2 + \mathbf{e}_3 & \dots & \mathbf{U}_i + \mathbf{e}_3 & \dots & \mathbf{U}_{2^k} + \mathbf{e}_3 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \mathbf{e}_j & \mathbf{U}_2 + \mathbf{e}_j & \dots & \mathbf{U}_i + \mathbf{e}_j & \dots & \mathbf{U}_{2^k} + \mathbf{e}_j \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \mathbf{e}_{2^{n-k}} & \mathbf{U}_2 + \mathbf{e}_{2^{n-k}} & \dots & \mathbf{U}_i + \mathbf{e}_{2^{n-k}} & \dots & \mathbf{U}_{2^k} + \mathbf{e}_{2^{n-k}} \end{array}$$

The all-zeros codeword $\mathbf{U}_1$ plays two roles. It is one of the codewords and it can also be thought of as the error pattern $\mathbf{e}_1$ – the pattern that represents no error, such that $\mathbf{r} = \mathbf{U}$. The array contains all 2^n n -tuples in the space V_n . Each n -tuple appears in *only one* location – none is missing, and none is replicated. Each coset consists of 2^k n -tuples. Therefore, there are $\binom{2^n}{2^k} = 2^{n-k}$ cosets [1].

The decoding algorithm calls for replacing a corrupted vector (any n -tuple excluding those in the first row) with a valid codeword from the top of the column containing the corrupted vector. Suppose that a codeword $\mathbf{U}_i$ ($i=1, \dots, 2^k$) is transmitted over a noisy channel, resulting in a received corrupted vector $\mathbf{U}_i + \mathbf{e}_j$. If the error pattern $\mathbf{e}_j$ caused by the channel is a coset leader, where the index $j=1, \dots, 2^{n-k}$, the received vector will be decoded correctly into the transmitted codeword $\mathbf{U}_i$. If the error pattern is not a coset leader, then the decoding will be erroneous. If $\mathbf{e}_j$ is the coset leader or error pattern of the j^{th} coset, then $\mathbf{U}_i + \mathbf{e}_j$ is an n -tuple in this coset. The syndrome of this n -tuple can be written $\mathbf{S} = (\mathbf{U}_i + \mathbf{e}_j)\mathbf{H}^T = \mathbf{U}_i\mathbf{H}^T + \mathbf{e}_j\mathbf{H}^T$. Since $\mathbf{U}_i$ is a code vector and $\mathbf{U}_i\mathbf{H}^T = \mathbf{0}$, then $\mathbf{S} = (\mathbf{U}_i + \mathbf{e}_j)\mathbf{H}^T = \mathbf{e}_j\mathbf{H}^T$. The name *coset* is short for “a set of numbers having a common feature.” Each member of a coset has the same syndrome. The syndrome for each coset is different from that of any other coset in the code; it is the syndrome used to estimate the error pattern [1].

The procedure for error correction decoding proceeds as follows: 1) Calculating the syndrome of $\mathbf{r}$ using $\mathbf{S} = \mathbf{r}\mathbf{H}^T$. 2) Locating the coset leader (error pattern) $\mathbf{e}_j$, whose syndrome is equal to $\mathbf{r}\mathbf{H}^T$. This error pattern is assumed to be the corruption caused by the channel. The corrected received vector, or codeword, is identified as $\mathbf{U} = \mathbf{r} + \mathbf{e}_j$. The valid codeword is retrieved by subtracting out the identified error; in modulo-2 arithmetic, the operation of subtraction is identical to that of addition.

Returning to the example in Table 1, the $2^6 =$ sixty-four 6-tuples are arranged in a standard array as shown in Fig. 2. The valid codewords are the eight vectors in the first row, and the *correctable error patterns* are the seven nonzero coset leaders in the first column. All 1-bit error patterns are correctable. After exhausting all 1-bit error patterns, there remains some error-correcting capability since all sixty-four 6-tuples have not yet been accounted. There is one unassigned coset leader; therefore, there remains the capability of correcting one additional error pattern. There is the flexibility of choosing this error pattern to be any of the n -tuples in the remaining coset. In Fig. 2 this final correctable error pattern is chosen, somewhat arbitrarily, to be the 2-bit error pattern 010001. Decoding will be correct if, and only if, the error pattern caused by the channel is one of the coset leaders.

000000	110100	011010	101110	101001	011101	110011	000111
000001	110101	011011	101111	101000	011100	110010	000110
000010	110110	011000	101100	101011	011111	110001	000101
000100	110000	011110	101010	101101	011001	110111	000011
001000	111100	010010	100110	100001	010101	111011	001111
010000	100100	001010	111110	111001	001101	100011	010111
100000	010100	111010	001110	001001	111101	010011	100111
010001	100101	001011	111111	111000	001100	100010	010110

Fig. 2. Example of a standard array for a (6, 3) code

The syndrome corresponding to each of the correctable error sequences is determined by computing $\mathbf{e}_j\mathbf{H}^T$ for each coset leader, as follows:

$$(18) \quad \mathbf{S} = \mathbf{e}_j \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix}.$$

The results are listed in Table 2. Since each syndrome in the table is unique, the decoder can identify the error pattern $\mathbf{e}$ to which it corresponds.

Table 2. Syndrome Look-Up Table

Error pattern	Syndrome
000000	000
000001	101
000010	011
000100	110
001000	001
010000	010
100000	100
010001	111

The vector $\mathbf{r}$ is received and its syndrome is calculated using $\mathbf{S} = \mathbf{r}\mathbf{H}^T$. Then the syndrome look-up table (Table 2) is used to find the corresponding error pattern. This error pattern is an estimate of the error, and it is denoted as $\hat{\mathbf{e}}$. The decoder then adds $\hat{\mathbf{e}}$ to $\mathbf{r}$ to obtain an estimate of the transmitted codeword $\hat{\mathbf{U}}$:

$$(19) \quad \hat{\mathbf{U}} = \mathbf{r} + \hat{\mathbf{e}} = (\mathbf{U} + \mathbf{e}) + \hat{\mathbf{e}} = \mathbf{U} + (\mathbf{e} + \hat{\mathbf{e}}).$$

If the estimated error pattern is the same as the actual error pattern, i.e. $\hat{\mathbf{e}} = \mathbf{e}$, then the estimate $\hat{\mathbf{U}}$ is equal to the transmitted codeword $\mathbf{U}$. If the error estimate is incorrect, the decoder will estimate a codeword that was not transmitted, and there is an *undetected decoding error*.

Assume that codeword $\mathbf{U} = 101110$ is transmitted, and the vector $\mathbf{r} = 001110$ is received. Show how a decoder, using the Table 2 syndrome look-up table, can correct the error. The syndrome of $\mathbf{r}$ is computed:

$$(20) \quad \mathbf{S} = [0 \ 0 \ 1 \ 1 \ 1 \ 0]\mathbf{H}^T = [1 \ 0 \ 0].$$

Using Table 2, the error pattern corresponding to the syndrome above is estimated to be $\hat{\mathbf{e}} = 100000$. The corrected vector is then estimated by

$$(21) \quad \hat{\mathbf{U}} = \mathbf{r} + \hat{\mathbf{e}} = 001110 + 100000 = 101110.$$

Since the estimated error pattern is the actual error pattern in this example, the error correction procedure yields $\hat{\mathbf{U}} = \mathbf{U}$.

When the code is short as in the case of the (6, 3) code described here, the decoder can be implemented with simple circuitry. The steps that the decoder must take: (1) calculate the syndrome, (2) locate the error pattern, and (3) perform modulo-2 addition of the error pattern and the received vector (which removes the error). The circuit shown in Fig. 3 is made up of exclusive-OR (XOR) gates and AND gates that can accomplish the same result for any *single-error pattern* in the (6, 3) code. Based on Table 2, an expression for each of the syndrome bits can be written in terms of the received codeword bits as

$$(22) \quad \mathbf{S} = \mathbf{r}\mathbf{H}^T = \begin{bmatrix} r_1 & r_2 & r_3 & r_4 & r_5 & r_6 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix} \text{ and}$$

$$(23) \quad s_1 = r_1 + r_4 + r_6, \quad s_2 = r_2 + r_4 + r_5, \quad s_3 = r_3 + r_5 + r_6.$$

These syndrome expressions are used for wiring up the circuit in Fig. 3. The exclusive-OR gate is the same operation as modulo-2 arithmetic and hence uses the same symbol. A small circle at the termination of any line entering the AND gate indicates the logic COMPLEMENT of the signal [1].

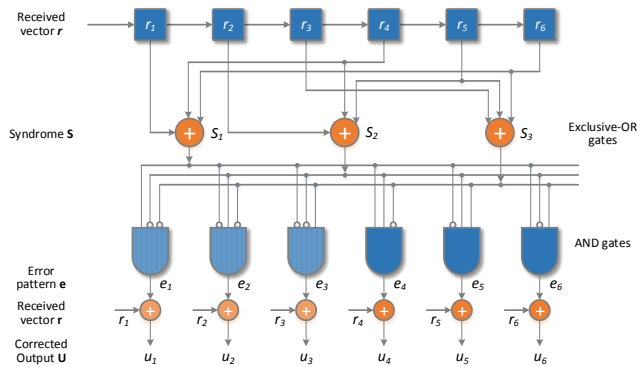


Fig. 3. Implementation of the (6, 3) decoder [1]

The corrupted signal enters the decoder at two places simultaneously. At the upper part of the circuit, the syndrome is computed, and at the lower part, that syndrome is transformed to its corresponding error pattern. The error is removed by adding it back to the received vector yielding the corrected codeword. Fig. 3 is drawn to emphasize the algebraic decoding steps – calculation of syndrome, error pattern, and corrected output. In the real world, an (n, k) code is usually configured in systematic form. The decoder would not need to deliver the entire codeword. Its output would consist of the data bits only. Fig. 3 circuitry becomes simplified by eliminating the gates shown with shading. For longer codes, such an implementation is very complex, and the preferred decoding techniques conserve circuitry by using a sequential approach instead of this parallel method. It is also important to emphasize that Fig. 3 has been configured to only detect and correct *single-error patterns* for the (6, 3) code. Error control for a double-error pattern would require additional circuitry.

4. Logisim – an educational tool for designing and simulating digital logic circuits

Logisim is an educational tool for designing and simulating digital logic circuits with simple toolbar interface. With the capacity to build larger circuits from smaller subcircuits, and to draw bundles of wires with a single mouse drag, Logisim can be used to design and simulate entire CPUs for educational purposes. Logisim is used by students at colleges and universities around the world in many types of classes. The main features of the product are: 1) It is free. 2) It runs on any machine supporting Java 5 or later; special versions are released for MacOS X and Windows. 3) The drawing interface is based on an intuitive toolbar. Color-coded wires aid in simulating and debugging a circuit. 4) The wiring tool draws horizontal and vertical wires, automatically connecting to components and to other wires. 5) Completed circuits can be saved into a file, exported to a GIF file, or printed. 6) Circuit layouts can be used as “subcircuits” of other circuits, allowing for hierarchical circuit design. 7) Included circuit components include inputs and outputs, gates, multiplexers, arithmetic circuits, flip-flops, and RAM memory. 8) The included “combinational analysis” module allows for conversion between circuits, truth tables, and Boolean expressions [3].

Features of the components used to build the encoder

The NOT gate emits the complement of the input it receives. The truth table for a NOT gate is the following [4]:

x	out
0	1
1	0

The AND, OR, NAND, and NOR gates compute the respective function of the inputs, and emit the result on the output.

By default, any unconnected inputs are ignored. In this way, a 5-input gate can be inserted but only two inputs are used, and it will work as a 2-input gate; this relieves the user from having to worry about configuring the number of inputs every time a gate is created. The two-input truth table for the gates is the following [4]:

x	y	AND	OR	NAND	NOR
0	0	0	0	1	1
0	1	0	1	1	0
1	0	0	1	1	0
1	1	1	1	0	0

The XOR, XNOR, Even Parity, and Odd Parity gates compute the respective function of the inputs, and emit the result on the output. By default, any inputs left unconnected are ignored. The two-input truth table for the gates is the following [4]:

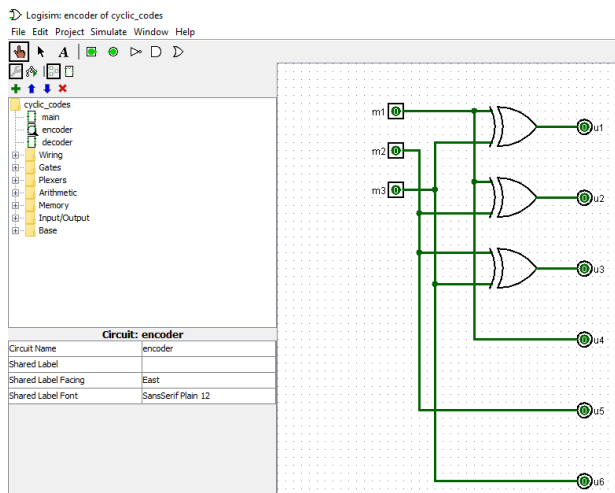
x	y	XOR	XNOR	Odd	Even
0	0	0	1	0	1
0	1	1	0	1	0
1	0	1	0	1	0
1	1	0	1	0	1

It seems that the Odd Parity gate and the XOR gate behave identically with two inputs; similarly, the Even Parity gate and the XNOR gate behave identically. If there are more than two specified inputs, the XOR gate will emit 1 only when there is exactly one 1 input, whereas the Odd Parity gate will emit 1 if there is an odd number of 1 inputs. The XNOR gate will emit 1 only when there is *not* exactly one 1 input, while the Even Parity gate will emit 1 if there is an even number of 1 inputs. The XOR and XNOR gates include an attribute titled Multiple-Input Behavior that allow them to be configured to use the Odd Parity and Even Parity behavior (Fig. 5). Many authorities contend that the shaped XOR gate’s behavior should correspond to the odd parity gate, but there is not agreement on this point. Logisim’s default behavior for XOR gates is based on the IEEE 91 standard. It is also consistent with the intuitive meaning underlying the term *exclusive or* [4].

5. Application in the Educational Process

The material is used in the educational process in the courses “Coding in Telecommunication Systems”, “Digital Circuits” and “Pulse and Digital Devices” included in the curriculum of the specialties “Internet and Mobile Communications”, “Computer Systems and Technologies”, “Computer Management and Automation”, “Electronics” and “Information and Communication Technologies” for the students of the Bachelor degree in the University of Ruse. In order to better perception of the material active learning methods are applied. An individual assignment is given to each student and he/she has to solve the task during the practical exercise and present it at the end of the classes to the lecturer. The student should synthesize an encoder and a decoder of a linear block code with XOR, NOT and AND gates and to simulate their operation using Logisim.

The circuits of the encoder and the decoder of a (6, 3) linear block code (Table 1, Fig. 3) are drawn and tested in Logisim, to verify their operation. The circuit is built by inserting in the editing area its components – 2-input or 3-input XOR gates ($\boxtimes$ XOR Gate), NOT gates ($\neg$ NOT Gate) and AND ($\boxdot$ AND Gate) gates first as a sort of skeleton and then connecting them with wires. To add inputs and outputs into the diagram, the Input tool ($\blacksquare$) and the Output tool ($\bullet$) are selected and the pins are placed down. The operation of the encoder and the decoder (Table 1, Fig. 3) is illustrated in Fig. 4 and Fig. 6. The results in Fig. 4 and Fig. 6 are identical to Table 1, Fig. 2 (the cells marked) and Fig. 3.



a)

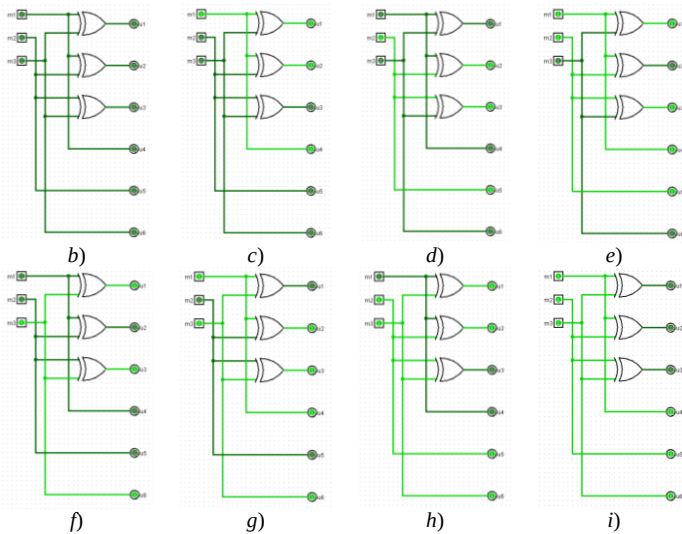


Fig. 4. a) Logisim and its simple toolbar interface + the circuit of the encoder (initial state – all-zeros) and encoding the message ...; b) 000; c) 100; d) 010; e) 110; f) 001; g) 101; h) 011; i) 111

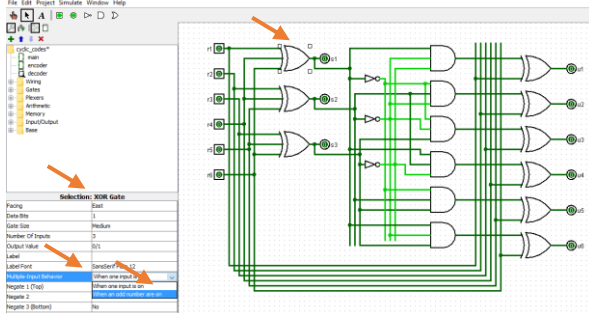
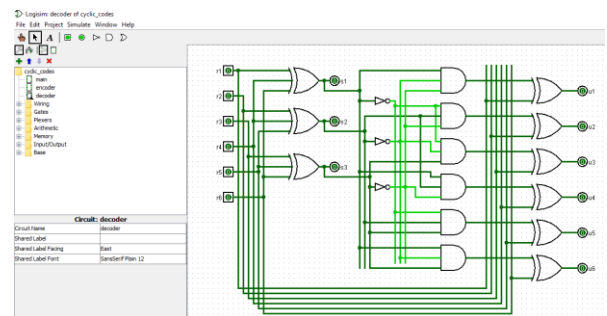


Fig. 5. Using the attribute Multiple-Input Behavior allowing the XOR gate to be configured to use the Odd Parity behavior

6. Conclusion

In order to easily assimilation of the material studied by students, active learning methods are applied in the educational process. An individual assignment is given to each student. The assignment includes: 1) filling in the blanks for a given encoder of a (6, 3) linear block code (Table 1, Table 2), after writing down the generator matrix and the parity-check matrix of the code given, implementing the decoder of the code given (Fig. 3); 2) synthesizing the encoder and the decoder of the (6, 3) linear block code with XOR, NOT and AND gates and simulating their operation using Logisim (Fig. 4 and Fig. 6). During the practical exercises, the student must solve his/her tasks of pre-prepared form published in the e-learning platform of the University of Ruse and submit to the teacher at the end of the classes. The opportunity for

extra work is given to the curious students – for example, synthesizing the encoder and the decoder of a (8, 4) linear block code using XOR, NOT and AND gates and simulating their operation using Logisim.



a)

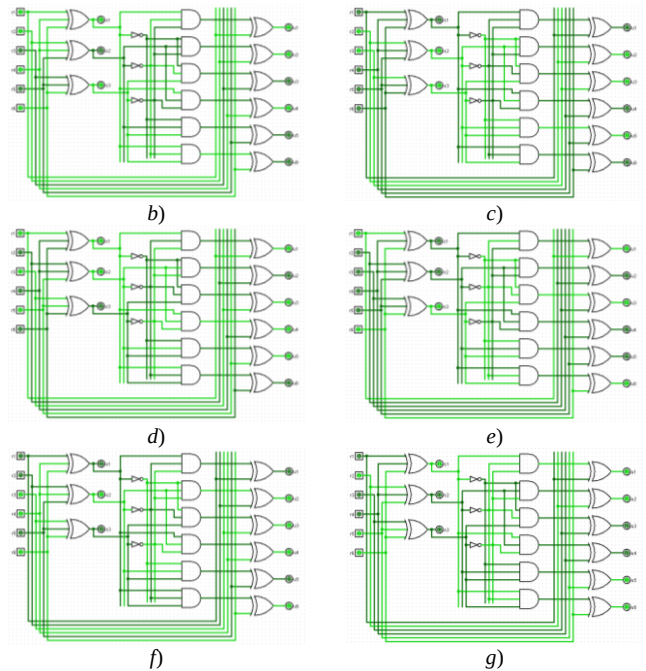


Fig. 6. a) Logisim and its simple toolbar interface + the circuit of the decoder (initial state – all-zeros); b) 110101; c) 011000; d) 101010; e) 100001; f) 001101; g) 010011

The study was supported by contract of University of Ruse “Angel Kanchev”, № BG05M2OP001-2.009-0011-C01, “Support for the development of human resources for research and innovation at the University of Ruse “Angel Kanchev””. The project is funded with support from the Operational Program “Science and Education for Smart Growth 2014-2020” financed by the European Social Fund of the European Union.

7. References

1. Sklar, B. Digital Communications. Fundamentals and Applications. Second Edition. Communications Engineering Services, Tarzana, California, 2001. http://userspages.uob.edu.bh/mangoud/mohab/Courses_files/sklar.pdf (visited in November 2017).
2. https://en.wikipedia.org/wiki/Linear_code (last visited in November 2017).
3. www.cburch.com/logisim/ (visited in November 2017).
4. Logisim Documentation (11 October 2014).

ELECTRIC POWER SYSTEMS MODELING AND EDUCATION: SHORT TERM UNIT COMMITMENT AND ECONOMIC DISPATCH MODELING FRAMEWORK

M.Sc. Trashlieva V.¹, M.Sc. Radeva T. PhD.¹

Department of Electrical Power Engineering – Technical University of Sofia, Bulgaria
vesselina.trashlieva@gmail.com

Abstract: In this paper we try to build a framework in optimization model building for students without previous mathematical optimization training and experience. While modeling is a matter of art, approach and compromise between complexity and closeness to reality we need to spend some time on the basics of optimization modeling such as cost function, constraints, variables and coefficients. There is a huge variety of optimization problems solved in Electric Power Systems. The most complex of all is considered to be the Unit Commitment problem where at each iteration an Economic Dispatch is performed.

Keywords: OPTIMIZATION MODELING, ELECTRIC POWER SYSTEMS OPTIMIZATION

1. Introduction

Students mastering Electric Power Systems (EPS) often have no previous mathematical modeling and optimization experience but are required to solve certain optimizations problems for EPS operation. Such problems are the Unit commitment (UC) problem and the Economic dispatch (ED) problem. The UC is an optimization problem used to determine the operation schedule of the generating units at every hour interval with varying loads under different constraints and environments[1]. At each hour the output power of each generator is determined via a solution to an ED problem. An ED is the problem for determining the power output of each power plant, and power output of each generating unit within a power plant, which will minimize the overall cost of fuel needed to serve the system load [2]. In an optimization problem the goal to achieve might be a single or a multiple criteria formulation, or multiple criteria may be combined together in a single cost function. There are also two big groups of optimization problems concerning the implicit existence of constraints: constrained and unconstrained optimization problems. In EPS modeling constraints are often present describing the process dynamics and the physics of the systems' components. Using Lagrange multipliers a constrained problem may be transformed into an unconstrained one leading to a general nonlinear unconstrained optimization problem. The latter is very sensitive to initial conditions while nonlinear functions seem to have more than one local extreme values and most of the methods for solving nonlinear problems find a local not a global extreme. The inconvenience of providing initial values for the search method and the fact that the risk of finding a local extreme not the global one make the Linear Programming approach a leading one in EPS optimization modeling. Linear (affine) functions have only one minima and maxima that are global and provides for the omission of second order Karush-Kuhn-Tucker conditions acquisition. Certain binary modeling techniques provide for the modeling of a set of important nonlinearities that often appear in practice while the resulting problem is still linear. Cost function and constraints may be linear or nonlinear functions, variables under consideration may be continuous, integer or binary, bounded or unbounded.

So all these matters and topics presented in the last paragraph determine the opulence of approaches and methods for optimization problems solving. This same richness requires a systematic approach in the processes and elements presentation in the mathematical model [3-6].

2. EPS model elements

When optimizing the performance of the EPS the respective power levels of the different power plants and loads are considered. To present the amount of active power produced by a certain power plant a continuous variable is used. These are optimization variables with general lower and upper bounds resulting from the real plant's capacity. If different states in the power plant's operation are possible integer and binary variables come at hand to represent the different operation states. Such states are for example "on" and "off"

or a role in frequency control reserve: "primary", "secondary" and "tertiary". Generally the set of all possible states is a closed one, meaning it includes a finite number of elements. In practice, binary variables have proven themselves as the most convenient for power plants' states representation leaving the space for general integer variables for other purposes. When the set of all possible states includes more than two elements it can be divided in more than one binary sets. For example, a pump hydro-power station can be idle (non-operational because of a fault, a planned repair or simply because its power is not needed in the power balance), can work as a load or as a generator. These three states can be presented with three numbers: -1 for pump, 0 for idle, 1 for generator. Two of these states coded with non-zero numbers (-1 and 1) can be further represented with binary variables with logical ones for true and zeroes otherwise. It is obvious that with such approach of breaking the initial set into few binary sets there is an overlap with the two binary sets' false values and the zero state in the initial set. So such breaking technique must be used very cautiously in order not to achieve a redundancy of binary variables that make problem solving more difficult.

Branch and bound and branch and cut are the contemporary techniques for solving mixed-integer optimization problems while the relaxed solution might be achieved via different optimization methods. No matter of the algorithm used, branching is an exhaustive process so the number of the integer and binary variables make the problem solving more complex and time spending according to the number of possible integer states. This is the reason that a trend towards integer and binary variables number as well as the number of the possible integer values reduction exists in order to make the branching easier and faster.

General integer variables are mostly used in EPS modeling when there are more than one system elements with similar features. In certain cases different power plants might be grouped according to common or similar characteristics: type or costs for fuel, similar working ranges, etc. This is another manifest of the latter approach for an overall variables reduction that provides for the usage of a single variable for the whole group of plants while the participation of each element of a group is a matter of a different optimization problem (ED). This ED might be nonlinear and will not include binary or integer variables, so its solving is generally more easy. Practitioners in EPS optimization modeling often use such approach in order to reduce the number of variables.

In EPS optimization modeling the variables are:

- integer and continuous according to their feasible sets;
- real and artificial according to the nature of physical processes they represent: real variables model real powers, loads and volumes, while artificial variables model states and alternatives;
- optimization and dual according to the stage of analysis;

3. Loads modelling

Some loads are controllable and others are not. From the systems' point of view controllable loads *help* for the power balance while the fixed loads *determine* a part of power balance. The work of the uncontrollable (fixed) loads might be forecasted and they participate in power balance constraints as forecasted values on the right-hand sides.

The controllable loads are as important as the generators are especially in the current renewable power generators penetration growth. Base power plants are not capable of flexible load following in both up and down directions. Wind and solar power stations are considered as stochastic uncontrollable base power plants so the power they might inject into the EPS is also considered as a forecasted value and unfortunately inject most of their power in low load hours. In high load hours peak power plants as hydro-power stations help for preserving the power balance. In other low load hours, the power of the base loads such as nuclear power stations need to be decreased and sometimes for wind and solar power stations even to be rejected if there is not enough load.

In detailed modeling terms controllable loads are considered in the following groups:

- controllable (dispatch) over time
- controllable over power level
- controllable over time and power level
- loads with interruptible or non-interruptible work cycle

For example a pump hydro-power station is a load that is dispatchable over time because pumps can be turned on when needed. A smart household appliance might be considered as a dispatchable over time load with a non-interruptible power cycle if it can not be stopped once started until the cycle is completed. In general, controllable loads modeling require the introduction of additional binary and integer variables.

4. Power plants operation modelling

According to the flexibility and the load following abilities generators are divided into two big groups: those of base and peak power plants. As mentioned above, there is one more aspect of power plants work namely if the output power level is controllable or stochastic. Wind and solar power stations are considered uncontrollable therefore their power generation is forecasted before the building and solving of the UC or ED problem [2]. These forecasted values participate as right hand sides along with the forecasts of the uncontrollable loads. All thermal, nuclear and hydro-power plants are considered controllable. The function representing the relation between spent amounts of fuels and produced power is generally non-linear because the electric power production process is nonlinear. These functions are often captured in practice with direct observations and in order to achieve a functional expression the appropriate function approximation techniques must be applied. Such experimental data is approximated with polynomials of order $N=2$ or 3 :

$$R(P) = \sum_{n=0}^N a_n P^n \quad (1)$$

Higher powers are suitable when higher precision is required or when inflexion points are more than 3. If the model has to be linear, a piece-wise approximation might also be used:

$$R(P) = \sum_{l=1}^L b_l P_l \quad (2)$$

In the latter expression $P = \sum_{l=1}^L P_l$ is the produced power in all

linear intervals $l = 1:L$, b_l is the fuel consumption growth in each consecutive interval l , and P_l is the power in the interval. So in a ED or UC optimization problem the number of continuous variables for each power plant that is modeled depends on the number of observation intervals, i.e. the value of L .

Table 1: Observed fuel consumption of a thermal power plant within its working range P_{min} – P_{max}

Interval l	$P_{l,min}$	$P_{l,max}$	b_l
	MW	MW	tons
	P_{min}	-	23,88
1	60	70	26,68
2	70	80	29,54
3	80	90	32,44
4	90	95	34,03
5	95	100	35,63
7	100	105	37,85
8	105	110	40,31
9	110	P_{max}	45,87

Given the data that is experimentally carried out for the fuel consumption of a power plant (Table 1, Figure 1), a piece-wise fuel consumption function may be used. In this case the number of variables increases with the increase of the number of observations.

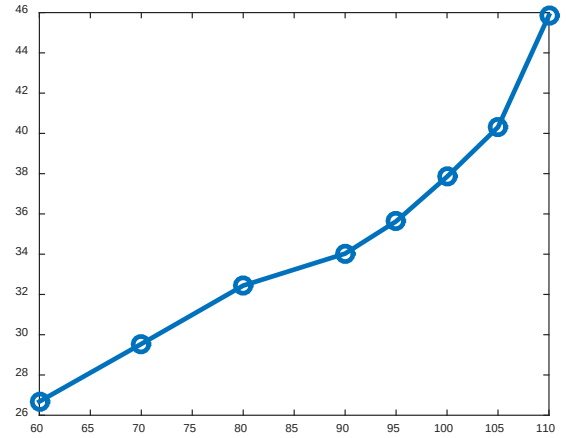


Fig. 1 Observed fuel consumption of a thermal power plant within its working range P_{min} – P_{max} graphical representation

A single continuous optimization variable may be used when the fuel consumption curve is nonlinear (1). Each point of this polynomial representation of a nonlinear function has its coordinates (P_n, b_n) . In this case an appropriate curve fitting procedure has to be used that minimizes the square of the difference between the real observation (P_l, b_l) and the evaluated one (P_n, b_n) in order to evaluate the values of the coefficients a_n bringing the polynomial approximation (1) closer to the observed values:

$$\min \sum [F(P_l) - R(P_n)]^2 \quad (3)$$

Because the cost function of the latter unconstrained optimization problem is nonlinear the appropriate initial conditions a_0 have to be provided for the problem optimization (3). As mentioned above the number n (i.e. the polynomial order N) of the coefficients whose value has to be optimized depends on the number of the inflexions of the initial data shown on Fig. 1. The procedure of curve fitting is performed only once whereas the observation data is stationary meaning that the values in the observations onto the fuel consumption do not change over time.

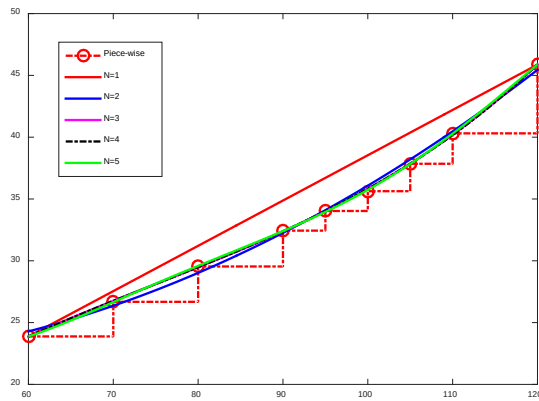


Fig. 2 Polynomial approximations of different orders

5. Costs structure and criteria

In optimization problems an optimal solution is found that fits best to certain criteria. In optimal power planning the most commonly used criteria is the minimal productions costs one. This is a variation of the minimal fuel costs (minimal raw materials consumption) criteria, that are determined by the consumption curve of each power plant. The fuel consumption curve multiplied by the price for the raw material (fuel) gives the fuel costs. These functions are generally nonlinear. Usually quadratic or polynomial approximations are used for the nonlinear case. In US problem on/off costs must be included. So two types of costs might be included in a cost function: costs that depend on the power plant's power level and costs that do not. This general idea for costs segregation introduces additional binary variables in the optimization models. More terms concerning different economic and financial relations may be also modeled as well as ecological criteria. All this makes the variety of cost functions wide enough to build different combined (multi criteria) goals.

6. Constraints

For the purpose of building a general idea and a modelling framework two large groups of constraints formulated in the optimization tasks in the EPS can be formulated. These are the system's conditions stating the balance requirement for each interval in the optimization horizon and the requirements for securing the reserves and the constraints arising from the production capacities. The second set of constraints may be further divided into subgroups according to the type of power plants (thermal, hydro), and a separate group of equality constraints responsible for water balances. Often in the optimization problems the working ranges of the plants are modelled by the simple bounds. Constraints that include efficiency coefficient η of the different cycles or mutually exclusive alternatives in the operation of units capable to work in reverse mode (pumps and turbines) form a separate subgroup:

minimize *Total Costs* subject to:

Balance constraints: $Production = Load + Losses$

Efficiency coefficient: $Accumulation. \eta = Generation$

Alternatives: $While\ true \leq Max\ variable\ value$

If false: Variable = 0

Water balance: *Waters used by pumps and turbines in different reservoirs and time intervals should equal or less than given constraints*

Simple bounds: $Min\ value \leq Variable \leq Max\ value$

Integer constraints: *Some variables are integer and ome variables are binary {0,1}*

On the other part constraints generally are represented mathematically with equations and inequalities. In optimization equality constraints are called *tight* or *binding* because every change in the right-hand side of an equality constraints leads to inevitable changes in the total costs. When there is an inequality constraints that is satisfied in the optimal solution as an equality this constraint is also *binding* because there is no *reserve* for changes in its right-hand side. Constraints also may be explicit or implicit in the formulation with implicit constraints being generally the possible sets of the values of all integer variables and the simple bounds arising from the working ranges while the latter may be easily included in the models constraints while the integer ones require further mathematical knowledge and work.

7. Conclusion

The presented topics above give general idea on EPS optimization modeling basics and possible points of view. A certain classification of power plants, loads and costs criteria is given. Some optimization modeling milestones are mentioned as well as few techniques to model size reduction are given.

8. Bibliography

- [1] Saravanan, B., Das, S., Sikri, S. et al., A solution to the unit commitment problem - a review, *Frontiers in Energy* (2013) Vol 7: pp. 223-226, <https://doi.org/10.1007/s11708-013-0240-3>
- [2] Wang J., Botterud A., Miranda V., Monteiro C., Sheble G., Impact of Wind Power Forecasting on Unit Commitment and Dispatch
- [3] Wang Y., Niu D., Ji L., Short-term power load forecasting based on IVL-BP neural network technology, *Systems Engineering Procedia* 4 (2012), p. 168 – 174, The 2nd International Conference on Complexity Science & Information Engineering
- [4] Usaola J., Castronuovo E. D., *Wind Energy in Electricity Markets with High Penetration*, Nova Science Publishers Inc, ISBN: 978-1-60741-153-6, 2009
- [5] Viana A., Pedroso J. P., A new MILP-based approach for Unit Commitment in power production planning, *International Journal of Electrical Power & Energy Systems*, Volume 44, Issue 1, January 2013, p. 997-1005
- [6] Vieira F., Ramos H. M., Hybrid solution and pump-storage optimization in water supply system efficiency: A case study, *Elsevier Energy Policy*, ISSN: 0301-4215, Volume 36, Issue 11, November 2008, Pages 4142-4148

ROBUST DESIGN AND MULTIPLE CRITERIA OPTIMIZATION OF ELECTRON BEAM GRAFTING OF CORN STARCH

Assoc. Prof. M.Sc. Eng. Koleva E. PhD.^{1,2}, M.Sc. Eng. Koleva L.², M.Sc. Eng. Nemțanu M.R. PhD.³, M.Sc. Brașoveanu M. PhD.³

Institute of Electronics, Bulgarian Academy of Sciences, Bulgaria¹

University of Chemical Technology and Metallurgy, Bulgaria²

National Institute for Lasers, Plasma and Radiation Physics, Electron Accelerators Laboratory, Romania³

eligeorg@abv.bg

Abstract: Electron beam (EB) irradiation has the ability to modify polymer substrates by process of graft copolymerization to synthesize water-soluble copolymers having flocculating potential. Models - depicting the dependencies of the described quality characteristics (their means and variances) from process parameters - are estimated by implementation of the robust engineering methodology for quality improvement. Multiple criteria optimization based on the desirability function approach, involving requirements for economic efficiency, assurance of low toxicity, high copolymer efficiency in flocculation process, good solubility in water, bias, robustness, quality of prediction and the relative importance of responses, is presented.

Keywords: GRAFT COPOLYMERIZATION, ELECTRON BEAM IRRADIATION, WATER-SOLUBLE COPOLYMERS, STARCH, ACRYLAMIDE, RESPONSE SURFACE METHODOLOGY

1. Introduction

The model-based robust approach for improving the quality of the process [1, 2] can be successfully applied to different industrial processes. For each of the quality performance characteristics, using their regression models, two other models are estimated - for their mean values and variances. The quality improvement is performed using some overall criterion or simply by the performance characteristics variances minimization, while keeping their mean values close to their target values. The Robust Parameter Design (RPD) is an issue of numerous papers in the literature since 1990 [3, 4], but there are much less of them in the area of application of RPD [1, 5] for multiple responses. Some of these articles consider the multi-response case, when replicated observations are available [6], while others are focused on formulation of appropriate optimization criteria. A systematic procedure implementing response surface methodology and desirability function for optimization of multiple response surface (MRS) problems that accommodates all of bias, robustness and quality of prediction besides relative importance of responses in a single framework is developed in [7] and compared with other multiple response techniques.

Electron beam (EB) grafting is a process of modification of polymer substrates implementing radiation-induced graft copolymerization in order to yield water-soluble copolymers having flocculation abilities [8]. The irradiation was performed with linear electron accelerator of mean energy of 5.5 MeV, and the influence of the variation of the following parameters: acrylamide/starch (AMD/St) weight ratio, electron beam irradiation dose and dose rate was investigated. The characterization of graft copolymers was carried out by monomer conversion coefficient, %; residual monomer concentration, %; intrinsic viscosity, dL/g; and Huggins' constant.

In this paper the robust parameter design methodology is applied for estimation of models, describing the dependencies of the means and the variances of the investigated quality characteristics. Multiple criteria optimization based on the desirability function approach, involving requirements for economic efficiency, assurance of low toxicity, high copolymer efficiency in flocculation process, good solubility in water, bias, robustness, quality of prediction and the relative importance of responses, is presented.

2. Robust parameter design

EB modification of polymer substrates through radiation-induced graft copolymerization is generally used to develop a wide variety of ion exchangers, polymer-ligand exchangers, chelating copolymers, hydrogels, affinity graft copolymers and polymer electrolytes, having various applications in water treatment, chemical industry, biotechnology, biomedicine, etc. [9, 10].

The synthesized graft copolymers were characterized [8] by the following performance quality parameters: y_1 [%] - residual monomer concentration, y_2 [%] - monomer conversion coefficient, y_3 [dL/g] - intrinsic viscosity and y_4 - Huggins' constant. The variation regions $[z_{\min}-z_{\max}]$ of the process parameters were: EB irradiation dose (z_1) - [0.64 - 1.44 kGy]; the EB irradiation dose rate (z_2) - [0.45 - 1.40 kGy/min] and the (AMD/St) weight ratio (z_3) - [5.00 - 10.02]. The concentration of St for these experiments varies from 2.00% to 6.15% and the concentration of AMD varies from 10.00% to 33.67%.

The conducted experimental design consisted in 20 experimental process parameter sets [8]. For each set of the process parameters three replicated measurements were used for estimation of the means and the variances of the quality characteristics of the graft copolymers. The estimated values of the means $\bar{y}_u$ and the variances s_u^2 can be considered as two responses at the design points and ordinary least squares method can be used to fit regression models for the mean value and for the variance for each quality characteristic [1]:

$$\begin{aligned}\tilde{y}(\bar{x}) &= \sum_{i=1}^{k_y} \hat{\theta}_{yi} f_{yi}(\bar{x}) \\ \ln(\tilde{s}^2(\bar{x})) &= \sum_{i=1}^{k_\sigma} \hat{\theta}_{\sigma i} f_{\sigma i}(\bar{x}),\end{aligned}$$

where $\hat{\theta}_{yi}$ and $\hat{\theta}_{\sigma i}$ are estimates of the regression coefficients, and f_{yi} and $f_{\sigma i}$ are known functions of the process parameters x_i . The variance of normally distributed observations has a χ^2 -distribution. The use of the logarithm transformation of the variance function makes it approximately normally distributed, which improves the efficiency of the estimates of the regression coefficients.

The response surfaces models for the mean and standard deviation of the quality characteristic are estimated and presented in Table 1 for coded values of the process parameters in the region [-1÷1]. The coding of the process parameter values is done, using the following equation:

$$x_i = (2z_i - z_{i,\max} - z_{i,\min}) / (z_{i,\max} - z_{i,\min})$$

where x_i and z_i are the coded and the natural values of the process parameter, correspondingly, $z_{i,\min}$ and $z_{i,\max}$ are the minimal and the maximal values of the parameter experimental variation region.

Table 1: Models for the means and variances of the product quality characteristics

Parameter	Models	R ²	W ^t
$\tilde{y}_1(\bar{x})$	$1.8416958 - 1.4711672x_1 + 0.39465799x_2 + 0.76523861x_1^2 - 1.4618933x_1x_2$	0.8172	0.1652
$\tilde{y}_2(\bar{x})$	$89.612983 + 6.1859389x_1 + 2.921934x_3 + 5.2145372x_2^2 - 2.1297402x_1x_3$	0.7415	0.1499
$\tilde{y}_3(\bar{x})$	$4.2786392 - 0.95051438x_2 + 2.2118238x_3 + 1.2412826x_2^2 - 7.0991376x_1^2x_2 + 0.721455x_2x_3 - 1.2935142x_1^2x_3$	0.7921	0.1602
$\ln(\tilde{y}_4(\bar{x}))$	$0.86268086 + 1.5188592x_2 - 1.6109201x_3 + 0.87526587x_1x_3 - 1.6469938x_2x_3 + 1.4461714x_1^2x_3$	0.6191	0.1252
$\ln(\tilde{s}_1^2(\bar{x}))$	$-3.0237265 - 0.60469566x_2 - 1.0612263x_3 - 4.3482641x_1^2 - 4.2402799x_2^2 + 5.604919x_1x_2 - 2.2657548x_2x_3$	0.7179	0.1451
$\ln(\tilde{s}_2^2(\bar{x}))$	$0.09316988 - 1.0210062x_2 - 1.7785371x_3 - 4.6387008x_1^2 - 4.9999832x_2^2 + 6.047145x_1x_2 - 2.242544x_2x_3$	0.7550	0.1527
$\ln(\tilde{s}_3^2(\bar{x}))$	$-2.5452688 - 0.67825221x_3 - 2.7034767x_1^2 - 2.1048188x_2^2 + 3.2229606x_1x_2 + 0.88934159x_2^2x_3$	0.5028	0.1017

Table 2: Specification regions and target values for the mean values and the standard deviation of response variables

Bounds	$\tilde{y}_1(\bar{x})$	$\tilde{y}_2(\bar{x})$	$\tilde{y}_3(\bar{x})$	$\tilde{y}_4(\bar{x})$	$\tilde{s}_1^2(\bar{x})$	$\tilde{s}_2^2(\bar{x})$	$\tilde{s}_3^2(\bar{x})$
lb	0	90	6	0.3	0	0	0
ub	5	100	9	1	0.2	1.8	0.6
τ	smaller	larger	larger	0.6	smaller	smaller	smaller

In Table 1 the estimated response model's quality of prediction is measured by the squared multiple correlation coefficient R².

3. Desirability function approach

An approach for optimization of multiple responses simultaneously is combining them into a single function. The desirability technique analysis is presented by Derringer and Suich [11]. This approach includes systematic transform of the quality characteristic $\tilde{y}_j(\bar{x})$ into individual desirability function $d_j(\bar{x})$, calculated depending on the optimization tasks:

- cases with defined target values:

$$d_j(\bar{x}) = \begin{cases} \frac{\tilde{y}_j(\bar{x}) - lb_j}{\tau_j - lb_j}; & lb_j \leq \tilde{y}_j(\bar{x}) \leq \tau_j \\ \frac{\tau_j - ub_j}{\tau_j - lb_j}; & \tau_j < \tilde{y}_j(\bar{x}) \leq ub_j \\ 0; & \tilde{y}_j(\bar{x}) < lb_j \text{ or } \tilde{y}_j(\bar{x}) > ub_j \end{cases}$$

- cases the larger the better:

$$d_j(\bar{x}) = \begin{cases} 0; & \tilde{y}_j(\bar{x}) \leq lb_j \\ \frac{\tilde{y}_j(\bar{x}) - lb_j}{ub_j - lb_j}; & lb_j < \tilde{y}_j(\bar{x}) \leq ub_j \\ 1; & \tilde{y}_j(\bar{x}) \geq ub_j \end{cases}$$

- cases the smaller the better:

$$d_j(\bar{x}) = \begin{cases} 1; & \tilde{y}_j(\bar{x}) \leq lb_j \\ \frac{ub_j - \tilde{y}_j(\bar{x})}{ub_j - lb_j}; & lb_j < \tilde{y}_j(\bar{x}) < ub_j \\ 0; & \tilde{y}_j(\bar{x}) \geq ub_j \end{cases}$$

In this way the individual optimization desirability functions of the mean values of each response (d_{oj}) scaled in the region between 0 and 1 can be calculated, together with the individual robustness desirability functions (d_{rj}) [7]. Here lb_j and ub_j are the minimal and the maximal acceptable levels for the mean responses and the standard deviations, τ_j is the target or the desirable value of the j -th

quality characteristic (Table 2). The robustness here refers to the low sensitivity of the quality characteristics to the noise factors. This can be achieved by a proper selection of values for the controllable process parameters, and can lead to a reduction for variance of the response in production conditions.

For the consideration of robustness in multiple response optimization problems, the following measures are defined [7]:

- Optimization desirability function D_{opt} , defined as the weighted geometric average of the individual optimization desirability functions:

$$D_{opt}(\bar{x}) = d_{o1}(\bar{x})^{w_{1\mu}} d_{o2}(\bar{x})^{w_{2\mu}} \dots d_{om}(\bar{x})^{w_{m\mu}};$$

- Robustness desirability function D_{rob} , defined as the weighted geometric average of the individual robustness desirability functions:

$$D_{rob}(\bar{x}) = d_{r1}(\bar{x})^{w_{1\sigma}} d_{r2}(\bar{x})^{w_{2\sigma}} \dots d_{rm}(\bar{x})^{w_{m\sigma}};$$

A multi-response optimization problem requires an overall optimization, i.e. simultaneous satisfaction with respect to the mean and standard deviation of all of the quality characteristics by using a combined desirability function between optimization and robustness. The overall desirability function can be defined as follows:

$$D_{overall}(\bar{x}) = D_{opt}(\bar{x})^{w_{opt}} D_{rob}(\bar{x})^{w_{rob}}.$$

In order to formulate weights for a given magnitude of predictive capability, a relationship between the weights and a predictive capability index (squared multiple correlation coefficient, R²) is needed (see Table 1):

$$w_j = \frac{R_j^2}{\sum R_j^2}.$$

4. Optimization results and discussion

The overall desirability function in the considered EB induced synthesis of graft copolymers is calculated by:

$$D_{overall}(\bar{x}) = d_{o1}(\bar{x})^{w_{1\mu}} d_{o2}(\bar{x})^{w_{2\mu}} d_{o3}(\bar{x})^{w_{3\mu}} d_{o4}(\bar{x})^{w_{4\mu}} d_{r1}(\bar{x})^{w_{1\sigma}} d_{r2}(\bar{x})^{w_{2\sigma}} d_{r3}(\bar{x})^{w_{3\sigma}}$$

The acceptable specification regions and the type of the case for the individual desirability functions (target value, the larger the better, the smaller the better) are presented in Table 2.

Desirability functions are formulated for several cases:

Case 1: Without consideration of the models predictive capabilities, the weights w_j are their optimization and robustness geometric average degrees:

$$w_{o1} = w_{o2} = w_{o3} = w_{o4} = 1/4 \text{ and } w_{r1} = w_{r2} = w_{r3} = 1/3; \\ w_{opt} = w_{rob} = 1/2.$$

Case 2: With consideration of the models predictive capabilities, the weights w_j are calculated in Table 1.

Case 3: Without consideration of the models predictive capabilities the weights w_j are calculated, considering the mean and variances as equivalent functions by their geometric average degrees:

$$w_{o1} = w_{o2} = w_{o3} = w_{o4} = w_{r1} = w_{r2} = w_{r3} = 1/7;$$

Case 4: Without consideration of the models predictive capabilities, the weights w_j are equal [7]:

$$w_{01} = w_{02} = w_{03} = w_{04} = w_{r1} = w_{r2} = w_{r3} = 1, w_{opt} = w_{rob} = 1.$$

Table 3: Optimal individual and overall desirability functions

Case	z_1	z_2	z_3	d_{01}	d_{02}	d_{03}	d_{04}	d_{r1}	d_{r2}	d_{r3}	$D_{overall}$
1	1.3800	0.45	7.7108	0.6016	1	1	0.9990	0.9964	0.9988	0.9843	0.9351
2	1.3560	0.45	7.7359	0.6165	0.9826	1	0.9980	0.9947	0.9982	0.9802	0.9176
3	1.3760	0.45	7.7108	0.6042	1	1	0.9960	0.9962	0.9988	0.9836	0.9271
4	1.3760	0.45	7.7108	0.6042	1	1	0.9960	0.9962	0.9988	0.9836	0.5889

Table 4: Optimal values of the means and variances of the product quality characteristics

Case	$\tilde{y}_1(\bar{x})$	$\tilde{y}_2(\bar{x})$	$\tilde{y}_3(\bar{x})$	$\tilde{y}_4(\bar{x})$	$\tilde{s}_1^2(\bar{x})$	$\tilde{s}_2^2(\bar{x})$	$\tilde{s}_3^2(\bar{x})$
1	1.9920	100.00	21.9203	0.6004	0.00072	0.0024	0.0094
2	1.9173	99.83	20.5134	0.6008	0.0011	0.0032	0.0119
3	1.9792	100.00	21.6812	0.5988	0.00077	0.0022	0.0098
4	1.9792	100.00	21.6812	0.5988	0.00077	0.0022	0.0098

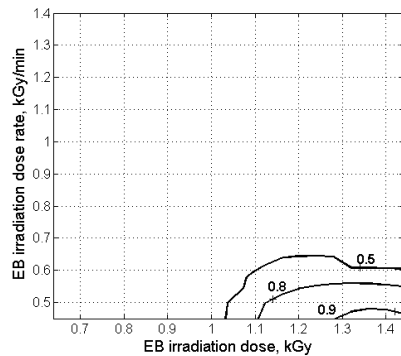


Fig. 1 Overall desirability function as a function of the process parameters EB irradiation dose (z_1) and the EB irradiation dose rate (z_2) at (AMD/St) weight ratio $z_3 = 7.7108$ – case 3.

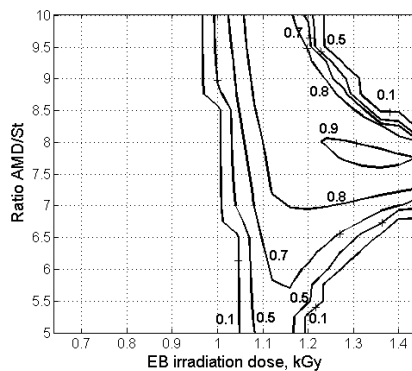


Fig. 2 Overall desirability functions as a function of the process parameters EB irradiation dose (z_1) and (AMD/St) weight ratio (z_3) at EB irradiation dose rate $z_2 = 0.45$ kGy/min – case 3.

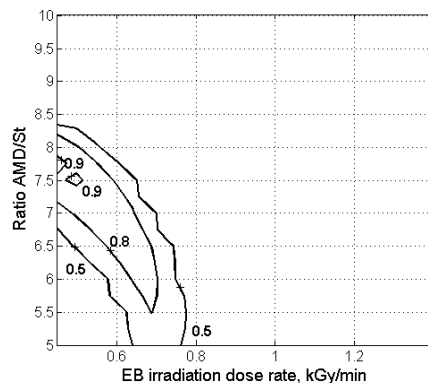


Fig. 3 Overall desirability functions, as a function of the process parameters EB irradiation dose rate (z_2) and (AMD/St) weight ratio (z_3) at EB irradiation dose $z_1 = 1.38$ kGy – case 3.

In Table 3 the individual (d_i) and overall desirability functions $D_{overall}$ are presented for the four considered cases, together with the obtained optimal process parameter values. The corresponding values of the estimated means and variances of the performance characteristics are shown in Table 4. It can be seen that there are no considerable differences in the obtained optimal process parameters and the means and variances of the quality characteristics, despite the differences in the calculated optimal overall desirability function values.

Fig. 1 – Fig. 3 display the contour plots of the overall desirability function as a function of different combinations of the process parameters: EB irradiation dose (z_1), the EB irradiation dose rate (z_2) and (AMD/St) weight ratio (z_3) for case 3.

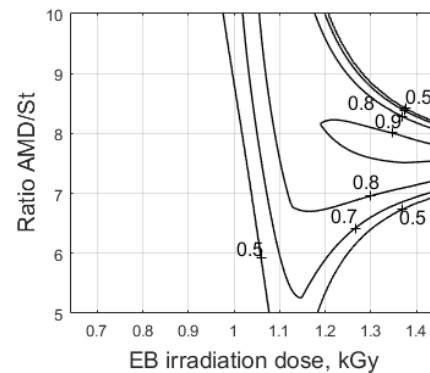


Fig. 4 Overall desirability functions as a function of the process parameters EB irradiation dose (z_1) and (AMD/St) weight ratio (z_3) at EB irradiation dose rate $z_2 = 0.45$ kGy/min – case 1.

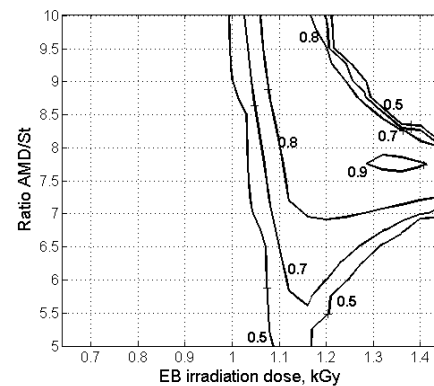


Fig. 5 Overall desirability functions as a function of the process parameters EB irradiation dose (z_1) and (AMD/St) weight ratio (z_3) at EB irradiation dose rate $z_2 = 0.45$ kGy/min – case 2.

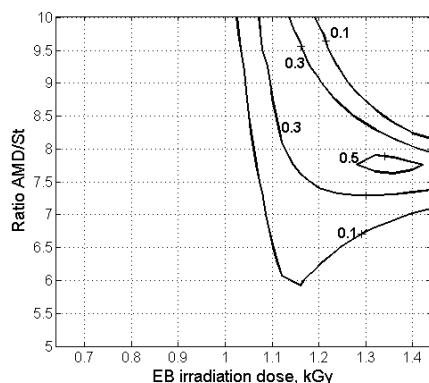


Fig. 6 Overall desirability functions as a function of the process parameters EB irradiation dose (z_1) and (AMD/St) weight ratio (z_3) at EB irradiation dose rate $z_2 = 0.45$ kGy/min – case 4.

Fig. 4 – Fig. 6 represent the contour plots of the overall desirability function as a function of the process parameters EB irradiation dose (z_1) and (AMD/St) weight ratio (z_3) at a constant value of the EB irradiation dose rate $z_2 = 0.45$ kGy/min for case 1, case 2 and case 4.

5. Conclusions

A multiple response optimization approach, based on overall desirability function, which considers the robustness as well as optimization of the process parameters at production conditions, is considered. Robustness and optimization desirability functions are calculated by evaluation of individual desirability functions of the means and variances of the product quality characteristics. The applied approach gives possibility to use weights for adjustment of the desirability functions according to the quality of model prediction and in favor of robustness or multiple response optimization.

Electron beam induced graft copolymerization used to synthesize water-soluble copolymers having flocculation abilities is investigated. The parameter optimization is performed in direction of fulfilling requirements for economic efficiency, assurance of low toxicity, high copolymer efficiency in flocculation process, good solubility in water, bias, robustness, quality of prediction and the relative importance of the quality characteristics.

Acknowledgements

This research was conducted under bilateral joint project between the Institute of Electronics at Bulgarian Academy of Sciences and the National Institute for Lasers, Plasma and Radiation Physics at the Romanian Academy. This work was also partially supported by a grant of the Romanian National Authority for Scientific Research, CNDI-UEFISCDI, project number 64/2012.

References

- [1]. Vuchkov I. N, Boyadjieva L. N. Quality improvement with design of experiments, The Netherlands, Kluwer Academic Publishers, 2001.
- [2]. Koleva E., I. Vuchkov, Model-based approach for quality improvement of EBW applications in mass production, Vacuum 77, 2005, pp. 423-428.
- [3]. Box G., S. Jones. Designing Products that are robust to the Environment. Quality and Productivity Report 56 Univ. of Wisconsin, CPQI, 1990.
- [4]. Vining G. G., R. H. Myers. Combining Taguchi and Response Surface Philosophies; A Dual-Response Approach. Journal of Quality Technology, 22, 1990, pp. 38-45.
- [5]. Myers R. H., D. C. Montgomery, G. G. Vining, C. M. Borror, S. M. Kowalski. Response Surface Methodology: A Retrospective and Literature Survey. Journal of Quality Technology, 36,1, 2004, pp. 53-77.
- [6]. Chiao C., M. Hamada. Analyzing Experiments with Correlated Multiple Responses. Journal of Quality Technology, 33, 2001, pp.451-465.
- [7]. Najafi S., A. Salmasnia, R. B. Kazemzadeh. Optimization of Robust Design for Multiple Response Problem. Australian Journal of Basic and Applied Sciences, 5(9), 2011, pp. 1566-1577
- [8]. Koleva E., L. Koleva, V. Tzotchev, M. Nemtanu, M. Braşoveanu, K. Vutova. Robust engineering approach for optimization of electron beam grafting of corn starch. Science, Engineering & Education, v.1(1), 2016, pp. 89-96.
- [9]. Stephen C. Lapin, Modification of Polymer Substrates using Electron Beam Induced Graft Copolymerization, UV+EB Technology • Issue 1, 2015, pp. 44-49.
- [10]. Nasef M.M., Radiation-grafted copolymers for separation and purification purposes: Status, challenges and future directions, Progress in Polymer Science, 37, 2012, pp. 1597– 1656.
- [11]. Derringer, G., R. Suich, Simultaneous optimization of several response variables. Journal of Quality Technology, 12, 1980, pp. 214-219.

TRAFFIC AND DRIVERS SYMBIOSIS: MANAGING BOTH FOR LOWER AIR POLLUTION

assistant professor dr. Angelevska B.¹, full professor Markoski A.², full professor dr. Atanasova V.³
Faculty of Technical Sciences^{1,3}, Faculty of information and communication technologies²,
University "St. Kliment Ohridski" Bitola, Macedonia
beti.angelevska@tfb.uklo.edu.mk, aleksandar.markoski@fikt.edu.mk, vaska.atanasova@tfb.uklo.edu.mk

Abstract: Air pollution problems in urban areas mainly can be connected with the high amounts of toxic exhaust emissions, generated from the growing use of vehicles that use fossil fuels [1]. Roads in urban areas are full with vehicles, and their management is important not just for smoothing traffic flows, but also for reduction of air pollution. Various ways could be considered in which traffic management can affect local air pollution [2]. But, is not just traffic management that should be considered solely. Attention should be given to the behavior of the drivers, which also has his impact on air pollution levels. Therefore, the purpose of this paper is to show the importance that traffic control and management as well as drivers' behavior together have on exhaust emission pollution. In addition to that, measures with their effects in the both categories: traffic management and drivers' behavior are proposed.

KEYWORDS: TRAFFIC CONTROL AND MANAGEMENT, DRIVERS' BEHAVIOR, AIR POLLUTION

1. Introduction

Growth of the number of vehicles, as well as the expansion of traffic systems are characterized with continuous trend [1]. Although emissions from new vehicles are less harmful than before, the roads in urban areas have become full with vehicles more than ever, most frequently with vehicles which are major air polluters. This concentration of vehicles makes urban air quality unpleasant and often harmful for breathing.

The rising amounts of road traffic emissions are connected with the increase of the fuel consumption in traffic and increase of traffic demand. Road transport presents an energy-consumption sector with a highest growth [1]. In a combination with the continuous growth of fuel consumption and the mileage per vehicle, the vehicles remain in the center of air pollution problem. Therefore, traffic management is important not just from the aspect of improvement of traffic conditions, but also from the aspect of air quality protection.

Although road traffic is a main contributor to air pollution [3], traffic management and drivers' behavior are often analyzed separately from each other. This paper makes an effort to present a comprehensive approach including both components and to suggest measures that could be employed to secure environmental benefits.

2. Traffic and air pollution

2.1. The impact of traffic management and control on air pollution

An efficient road traffic system is of high importance to every society [3]. Many local authorities face a challenging situation with a steady increase in road traffic, leading to congestion and longer travel times. This is happening despite the measures to reduce congestion, e.g. by improving the traffic control, implementing road toll and stimulating use of public transport and other sustainable alternatives. As a result of congestion, fuel consumption increases together with emissions. In particular during peak hours, the emissions found in cities often exceed acceptable local, national and European limits [3].

Traffic management comprises both "supply side" measures (traffic system management to improve speeds of existing traffic volumes) and "demand side" measures (traffic demand management to improve speeds by reducing traffic volumes).

For example, traffic management may require some physical measures, usually referred to as traffic engineering [2]. Improvements in urban infrastructure can result with a decrease in vehicle emissions, even in the case when all other factors will stay unchanged. But, the improved conditions for traffic flows can offer

only a short-term improvement in urban traffic and only a short-term emission reduction [1]. Uncontrolled vehicle growth, following the road infrastructure improvements, is a negative result on the efforts regarding improvements of urban air quality.

Another way of traffic control is through traffic signals. If this is used not just for smoothing traffic flows, but also for their orientation towards open roads (from one or both sides) where natural ventilation contributes for emission dispersion, the benefits for urban air quality are bigger. Additionally, traffic signal control can successfully promote public transport as more attractive solution, giving a priority in crossroads.

Contribution in emission reduction can be achieved using variable message signs to inform the drivers for the speed limitations, available parking places, traffic calming zones etc. Variable message signs, supported by intelligent system which continuously monitors and forecasts local pollution and dynamically controls traffic signals, can be especially effective for emission reduction. In comparison with the unchangeable speed limitations or signs, variable message signs are changeable during the day, as a response of the change in road and traffic conditions and variations in air pollutions.

In fact, every technology or measure that encourages common usage of vehicles, change in the way of usage of passenger vehicles, promotion of public transport, walking and cycling can reduce exhaust emissions.

2.2. Measures for traffic control and management for air pollution reduction

Measures for traffic control and management, which have a positive influence on vehicle exhaust emissions appears in many forms. Most often, they have an impact on traffic operational characteristic, on the way that vehicles have been used, on promotion of sustainable alternatives (public transport, walking, cycling). Numerous measures for traffic control and management are defined, with a potential for exhaust emission reduction, including parking control, park&ride, urban logistics, massive transit systems and improvements in public transport.

However, this kind of measures is faced with the following obstacles [1]:

- problems with the range of the impact – measures focused in central urban zones will have only a small impact on emissions in the broader areas
- political problems – some of the measures, such as increase of the taxes for road toll, fuel taxes and taxes in public transport, politically is very difficult to be implemented.

The following measures are presented in the form of table and could be considered for traffic control and management in order to

decrease high pollution episodes from exhaust emissions.

Table 1: Measures for traffic control and management

Measure	Effect
road toll	stimulation of modal change, especially if taxes are 2-3 times higher during the peak hours
synchronization of traffic signal control systems	green waves and reduced idling time
priority for high occupancy vehicles during the peak hours	reduction of the number of vehicles on urban roads
parking payment	modal change and decreased usage of the vehicles
limited entrance for the passenger vehicles and high duty vehicles in the city center	minimization of traffic volumes in city center and increase of the traffic speed
programs for limited expansion of the road space for motorized vehicles	increase of the road space for sustainable modes
traffic calming zones	modal change
public transport priority	modal change
priority for cyclist and walkers; safe crossing	modal change
de-leveled separation of the crossing with major roads	network without signal control (in the long- term)

Source: Made by the authors

Apart of these measures, especially should be emphasized the programs for car-free journeys and programs for decreasing the need for individual journey with a car, as the most significant components in traffic planning and control. Their realization is highly conditioned by the development of all less-polluting traffic alternatives.

Critical to the successful implementation of traffic management measures is the establishment of a traffic management unit at the local level with the ability to plan and implement suitable traffic management schemes [2].

Presented measures for traffic control and management from the aspect of air pollution reduction have a suggestive nature. Before their implementation, a detailed technical studies and research are needed. In any case, modern vehicle technologies and intelligent traffic systems have a significant potential for the solution of air pollution problems in the urban environment and development of sustainable traffic in urban areas [4].

3. Drivers' behavior and air pollution

The style of driving the vehicle has high impact on the amount of released exhaust emissions. The most important influence on emission levels for a given vehicle is the driving cycle, with both fuel consumption and pollutant emissions many times higher per vehicle km during acceleration and deceleration than during cruise [2].

Eco-driving is a driving style aimed at preventing environmental degradation by reducing fuel consumption and greenhouse gas emissions, which in turn saves money [5]. Eco-driving offers benefits for drivers of private cars, company cars, lorries and busses, as well as fleet owners. Eco-driving can assist in effectively reducing fuel consumption thereby reducing harmful vehicle emissions and pollutants such as CO₂ which is one of the greenhouse gases that contributes to the climate change [5].

Before proposing several practical advices how to properly eco-drive a vehicle to reduce exhaust emissions, attention is given to other aspects that contribute to the change in drivers' behavior.

These aspects are: drivers' information during the journey and informed buying of new vehicle.

3.1. Drivers' information system during the journey

Advanced information system for the drivers during the journey (GPS), for example by proposing optimal routes, reduces the necessary travelled mileage. In this way, indirectly contributes for the reduction in urban air pollution.

In-vehicles guidance systems provide real-time information for the location of the most congested and polluted places, advising the driver for the alternative routes. In most ideal case, drivers' information should include details for other travelling modes, for example by public transport, availability to the public transport and price, although drivers unwillingly accept public transport as an alternative for its own vehicle.

The use of these information systems imposes the need of more effective wide-range activities for data collection and their distribution to the drivers [1]. In-time and precise distribution of the collected data for air pollution are performed through networks for the surveillance of the level of polluted air and warning systems when the thresholds are exceeded, especially of particles, ozone, nitrogen oxides and sulfur oxides.

But, it must not be neglected that information system for the real situation with pollution levels, except that is helpful for the drivers, has another, even more important effect: contributes for the awareness of the broader public for the impact of traffic emissions on urban air quality. Hence, the system indirectly contributes for the increase of the pressure of the public for reduction of the vehicle emissions [1].

3.2. Informed choice for buying a new vehicle

The best individual contribution from every driver for emission reduction at local and global level could be achieved in the process of buying a new vehicle when an informed choice should be made [1]. Today, when much more is known for the relation between vehicle exhaust emissions and environmental pollution, it is

important that buyers of new vehicle know the consequences of their choice. The best solution is buyers to have available specific information about the environmental performances of the vehicles, so that a decision could be made based on better information.

Information when buying a new vehicle shouldn't be deduced only to the vehicle basic price, registration and insurance costs, maintenance costs of the additional equipment, performances, durability, safety etc. When buying a new vehicle, buyers should be informed also for the fuel consumption and costs, i.e., the total approximate cost for the fuel during the vehicle exploitation period, for the emission amounts of carbon dioxide and other exhaust emissions.

The data, that should be available when buying, most often are obtained during the official tests done before the car model has been offered for sale [1]. Very helpful could be the advices of the official distributors when choosing the most suitable way for reduction of vehicle impact on the environment. Classification of the vehicles in categories according to the environmental performances provides important information about the vehicle impact on air quality and the greenhouse effect.

When the choice is deduced to one selected class of vehicles (as the best according to the needs and opportunities), a vehicle that has a best fuel efficacy should be chosen. Unnecessary vehicle size and weight increase fuel consumption. For example, fuel consumption at vehicles with similar size could vary up to 45% [6].

Most of the countries have fiscal measures (most often referring the fuels) to stimulate the buyers to choose the vehicle with higher fuel economy and to stimulate drivers for eco-driving. Besides that, vehicles that use cleaner fuels and alternative fuels have additional discount [7].

3.3. Practical advices for the drivers for exhaust emission reduction

Every driver individually, taking some simple measures and changing his own habits during the driving, could significantly

contribute for the improvement of air quality and pollution reduction [1]. Emissions from every individual vehicle are really small, but because of the total global number of vehicles, an effect in pollution reduction could be achieved if every driver is keeping himself to some simple preventive measures for eco-driving.

Driver behavior has influence on fuel consumption and exhaust emissions; hence, a higher self-responsibility is needed. Moderation in the driving style is useful not just for the environment, but also helps in the continuation of the exploitation period at every component in the vehicle. Frequent stops and starts, aggressive deceleration and acceleration, bad vehicle maintenance often lead to the higher consumption and higher exhaust emissions [1].

Vehicle occupancy rate by several passengers are low and total distances passed with the vehicles are rising [1]. This change causes higher emission concentrations with negative influences on the environment. Although innovation at passenger vehicles has brought higher personal mobility, presenting a flexible and comfort way of personal transit, the current level of usage of passenger vehicles aren't sustainable. Hence, efforts for stimulating of alternatives such as walking, cycling and public transit should be putted. However, it is unreal to expect that the vehicle owners would give up of them preferring other alternative ways of transit [1].

The fact that every driver contributes for increases of the emissions, clearly indicates that should not be expected that only authorities have an obligation for undertaking measures for pollution reduction. For their politics to be effective and to provide realization of the anticipated goals, it is necessary every driver to act individually in the form of eco-driving style [1].

Several simple advices for the drivers that can contribute for the decrease of the vehicle impact on environment and for less air pollution are presented in table 2.

Table 2: Measures for drivers' behavior and eco-driving

Measure	Effect
use of a vehicle with low fuel consumption	decrease of the amount of exhaust emissions
avoidance of usage of the vehicle at short journeys	decreased exhaust emission per kilometer
previous planning of the journeys	selection of the optimal routes with low congestion and shorter travel time
car-pooling (more passengers in one vehicle)	decrease of the total number of vehicles on the urban roads
driving with lower speed	decrease of the fuel consumption and emission reduction
driving with constant speed without frequent accelerations and decelerations	fuel savings
preservation of the vehicle gap	fuel savings
avoidance of the constant breaks usage	fuel savings
regular maintenance of the vehicle	fuel savings and emission reduction
keeping the suitable tire pressure	fuel savings
rare usage of the air-conditioner	fuel savings

Source: Made by the authors

Local, as well as global pollution would have been significantly improved if every driver is disposed to use its own vehicle for 30% less than usual, starting from now. Bigger European cities could achieve real results in the environmental protection, if in the next 3-5 years the traffic of passenger vehicles is reduced for 30% [8].

These and other measures that modify drivers' behavior have the biggest potential for reduction of the total vehicle emissions [1].

4. Conclusion

Mobility needs in urban areas are constantly rising and most often the first choice for urban travel is passenger vehicle. The growth of the number of passenger vehicles on urban roads worsens the conditions of traffic flows, but also has very negative impact on urban air quality.

For dealing with this situation, a comprehensive approach is needed, taking into account traffic management and control and drivers' behavior. This means that from one side, a maximal effect in the traffic activities is necessary to be achieved. From the other side, special attention should be dedicated to the eco-driving style of the vehicles and changes in drivers' behavior in that direction. Eco-driving training is well-known as a feasible strategy to decrease fuel consumption and emissions [9].

Therefore, this analysis presents several measures together with their effects that can achieve reduction in air pollution during the congested traffic flowing on the road network, changing the drivers' behavior at the same time.

Traffic control and management is not a guaranteed, one-shot cure for traffic congestion. It needs constant adjustment and enforcement to be effective. Traffic management requires effective planning, implementation and enforcement skills [2].

Drivers' behavior has influence on fuel consumption and exhaust emissions; hence, a higher self-responsibility is needed. Following the eco-driving advices, every driver could contribute for decreasing of the local, as well as global emission levels.

Realization of the goal for significant reduction of emissions until 2030 it will be only possible by using an integrated approach which includes traffic management and control and changes in the way of driving (for reduction of the distances passed and fuel consumed). Also, the commitment of the authorities to maintain enforcement of proposed measures would be particularly critical [2].

References

- [1] Angelevska, B. Environmental impacts from passenger petrol car exhaust emissions. Master thesis. Faculty of Technical Sciences, University "St. Kliment Ohridski", Bitola, Macedonia, 2007, p. 102.
- [2] The World Bank. Urban air pollution. South Asia Urban Air Quality Management Briefing, Note No. 5, ESMAP, 2002, p. 4.
- [3] Gustafsson, S., Hübner, N., et al. Integration of traffic management and air quality control (iTRAQ). Association for European Transport and Contributors, 2012, p. 13.
- [4] Emission control technologies to meet future European vehicle emission legislation. International Conference on EUROV, Association for Emissions Control by Catalyst AECC, Milan, December 2003.
- [5] Air quality benefits of eco-driving. Western Cape Government, Environmental Affairs & Development planning. Cape Town, South Africa, p. 2.
- [6] Crépat, G. The road to a cleaner environment is a long one. Indoor Built Environ, Dijon, France, 1999.
- [7] Ghose, M.K. Controlling of motor vehicle emissions for a sustainable city. Centre of Mining Environment, Indian School of Mines, Volume 1, No. 2, June 2002.
- [8] Comparison of the EU and US experiences with respect for controlling emissions from high emitting vehicles. Case study 3, Assessment of the effectiveness of European air quality policies and measures, Project for DG environment carried out by Milien Lid, the Danish national environmental research institute and the Center for clean air policy, October 2004.
- [9] Yanzhi A.X., Hanyan A.L. et al. Eco-driving for transit. A white paper from the National center for sustainable transportation, Georgia Institute of Technology, College of Engineering, April 2016, p. 52.

TRAFFIC PRODUCTION MODEL USING MULTIPLE REGRESSION ANALYSIS AND RADIAL BASIS FUNCTION NEURAL NETWORK

*Prof.dr.Vaska Atanasova,¹, Mr.sc. Ramadan Duraku,², Associate prof.dr Beti Angjelevska³, Prof.dr.Nikola Krstanoski.⁴
Faculty of Technical Sciences, University "St.Kliment Ohridski", Bitola, Macedonia^{1,3,4}
Faculty of Mechanical Engineering, University of Prishtina "Hasan Prishtina", Prishtina, Kosovo²
(* Corresponding author: vaska.atanasova@tfb.uklo-edu.mk)

Abstract: In order to establish this model, several independent variables of aggregate level and dependent variables have been taken into account for traffic production of a region for a period of 24 hours. The objective of this paper is to identify and estimate the main variables which are significant for development of a suitable model for forecasting the traffic production for Anamorava region. Establishment and assessment of a model will be done using techniques such as Multiple Regression Analysis (MRA) and Radial Basis Function Neural Network (RBFNN). The results gained according to these two techniques will be compared to find out differences. In this regard performance analysis through indicators R^2 , ME, RSME which are also used to show errors in forecasting. The results are in favour of RBFNN model because it performs better than MRA in forecasting traffic production.

Keywords: TRAFFIC PRODUCTION, MODEL, MRA, RBFNN

1. Introduction

Transport planning process which is closely related to travel demand forecasting is essential for the design of transportation facilities and services, and also for planning, investment and policy making [1]. The models of forecasting in transport planning are very important to foresee increase of traffic and trips in the future. [2]. The traffic production modelling is to be done by finding relation between traffic countings which exit from a zone from origin - destination survey result and other independent variables of macro level in a given zone. This was a reason to undertake field research to find out the matrix origin-destination of traffic production for a period of 24 h treated here like independent variable in the Anamorava region. Later by application of various modelling techniques like those traditional –linear regression and those non traditional-RBFNN it will be possible to built a model for forecasting of traffic production.

1.1 The Objectives of the study

The objectives of this paper are: 1. Development of a suitable model for forecasting traffic production in Anamorava region using techniques such as MRA and RBFNN, and (2) comparison of results according models MAR and RBFNN by application of performance indicators like R^2 , ME and RSME.

2. Materials and methods

The methodology of traffic forecasting in this paper is addressed in three parts: (a) Data collection, (b) Regression models and (c) ANN models.

3.1 Data collection

In order to establish the model, the requirement was to identify and collect data on independent variables as well as dependent variables. Collection of data for variables which will be incorporated in setting up models is done according to two ways explained as follows.

2.1.1 Aggregate data

Demographic, economic and terrain factors have been taken like independent variables in aggregate level of more impact. Relevant data on this issue have been taken from competent authorities for collection, maintenance and archiving them [3], [4], [5] etc. Selection of independent variables is done in line with relevant literature [6], [7], [8] and [9]. Exclusion from this is on some territorial variables such is distance and time and the other one which is the result of them namely, cost of trip which is done by an author based on primary information available in Google maps etc.

2.1.2 Field data for traffic counting

The key place in this paper is the traffic produced on daily basis by this region qualified like independent variables (Y). Data on them is found out through the research conducted specifically for this purpose. The outcome of this is a matrix O-D of trips which is very important to proceeds with further steps towards establishment of a relation between variables and finally to establish models. This is made possible by completing manual counting and interviews in cordon in eight selected locations in the main road network with higher traffic flow in region. Forms and special questionnaires are prepared in advance to complete counting and interviews, which contain direction of trip (O-D), purpose of trip, frequency of trips, number of passengers in vehicle etc. Depending on origin and the purpose of trip we took into consideration internal-external, external-internal, internal-internal and transit traffic. The traffic within one zone was not subject of research. Counting and interviews are completed simultaneously on 18.05.2016 and 21.05.2016 non-stop for 12 hours starting from 07:00 am until 19:00 pm. There are 11523 interviews completed which is 19.43% of total traffic flow in two directions which also show 59317 vehicles counted manually. Counting and interviews are conducted assisted by students of Transport and Traffic Department supported by Kosovo Police.

2.1.3 Data Processing

After processing of data it was possible to establish the matrix O-D of real trips for each category of vehicles. Thus, knowing number of traffic flows and interviews conducted for a period of 12 hours and for only two days of the week, which is one working day and the other day is weekend, it was not possible to further continue without conducting additional calculation coefficients in relation to K_k , K_{int} and $K_{convert(12h/24h)}$ in order to gain final matrix of daily trips by vehicles. After counting is completed there is a need to correct them. Counting of traffic shows we have various types of vehicles which influence the traffic and requirement is to convert vehicles per unit in order to have uniform traffic influence. This measurement based on categories per vehicle will be converted to vehicles per unit equal to a car based on the equivalent coefficient value $K_k=1.4$. Gained values need to be multiplied with this coefficient to make the equivalent of PCSE.

2.1.3.1 The coefficient of interview

It is obvious that technically is not possible to interview every vehicle driver. In order to find the number of trips by vehicle within the period of 12 hours coefficient of interview K_{int} was used. This is gained comparing the traffic flow and the interviews conducted within given period of time for each location separately as given hereunder in equation 1 and results are presented in Table 1.

$$K_{int} = \text{No.vehicles}_{12h} / \text{No.interviews}_{12h} \quad (1)$$

Table 1: Interview coefficient

Location	Traffic volume veh/12h	Number of interview	%	Interview coefficient of vehicles (K_{int})
Slivovo	5494	1131	18.01	4.86
Sojevo	5981	1092	15.42	5.48
Begrac	3137	880	24.23	3.56
Kllokot	4749	925	17.73	5.13
Dheu i Bardhe	1148	278	57.43	4.14
Ranillug	5350	894	16.47	5.99
Livoc i Poshtem	7173	1354	18.41	5.30
Muqibabe	571	115	59.62	4.96

By using this coefficient, it was possible to establish of O-D trip matrix for total number of vehicles for a time interval of 12 hours applying equation 2 as follows:

$$\text{Matrix}_{O-D} = \text{No.interviews}_{12h} \cdot K_{int}[\text{veh}/12h] \quad (2)$$

2.1.3.2 Converting traffic from 12 h to 24 h

After processing the traffic flow conducted from automatic mobile counters for an interval of 24 hours which have been installed in four locations through it was possible to get converting coefficient of traffic from 12 hours to 24 hours through equation 3.

$$K_{\text{convert}(12/24)} = \text{No.vehicles}_{12h} / \text{No.vehicles}_{24h} \quad (3)$$

Comparison of data for four locations resulted in its average value is $K_{\text{convert}(12h/24h)} = 1.5$. In this regard, application of traffic flow values and values gained of these coefficients in equation 4, the final matrix is gained on O-D of trips of vehicles for the period of 24h.

$$\text{Matrix}_{O-D} = \text{Volume}_{12h} \cdot K_k \cdot K_{int} \cdot K_{\text{convert}12/24}[\text{veh}/24h] \quad (4)$$

This results from matrix is like an average of two days when counting and interviews are conducted with an intention not to require application of weekly nonlinear coefficient of trips.

4.2 Linear regression

In order to develop traffic production modelling, respectively to investigate relationship between of dependent variables Y_i and independent variables X_i , MRA technique is applied and this general form according to [10] is given in equation 5:

$$Y = \beta_0 + \sum_{i=1}^n \beta_i \cdot X_i + \varepsilon_i \quad (5)$$

Where: Y_i is number of productive trips per day, X_i -explanatory variable from 1 to n , β_0 is regression constant; β_i -is regression coefficient and ε_i -error.

Correlation coefficient is verified between every dependent variable with each independent variable in a specific way. According to this it results that demographic, economic and territorial phenomenon of various zones are well correlated ($R > 0.5$) with total number of trips. In this way we decided that each of them to include in analysis. The model is done using SPSS package software. Stepwise technique, backward and automatic linear regression were used to get the most statistical significance equations, between independent variables on dependent variable in the model [11]. After several attempts it was not possible to get the best results according to only "lin-lin" model and we needed to intervene in transformation of data in dependent variable applying several permitted ways of transformation shown in wide literature on statistics and econometric functions such as "log" [12]. Based on evidence it resulted that application of "log" in transformation of dependent variable provide best results compared to other functions. Selection of variables in final equation of regression is done following some principles as mentioned following: a. non existence of multi co-linearity between variables, b. variables need to be in harmony with engineering and logic judgement in relation to

developments, and c. selection of models with the less possible number of variables, to have in possession a history of series of variables taken for review, to have high value for determination of coefficient R^2 and low value of mean error (ME), root mean square error (RSME) [13].

5.3 ANN models

Artificial Intelligence technique is more frequently used in the last years for forecasting in many areas. Part of this technique is fuzzy logic, neural network, genetic algorithms, etc. [14]. All these three techniques are used for solving complicated problems at the same time and in combination. There is also a tendency to use ANN which is a tool to solve problems, which makes possible processing of data like input-output and the results are guaranteed in treating some inaccuracies while analytic equation of input-output are not needed.

ANN is a calculation model which is defined through the type of neuron, connection architecture, algorithm for learning etc. Based on connection architecture there are [15]: a. Feed forward which consist of: MLP, PNN, GRNN, CFN, RBF, AMN and b. Feedback which consist of Jordan Elman network-JENN, Hopfield network-HN, Adaptive resonance theory-ART, Recurrent network-RNN etc. Each of them has its own specifics and similarities to each other.

In this paper, the radial basis function neural network (RBFNN) model is provided. The methodology and parts of RBFNN models, variables and analysis used are described in the following discussion.

2.3.1 The topology of RBFNN

A radial basis function (RBFNN) is a feed-forward, supervised learning network with only one hidden layer, called the radial basis function layer. The RBF network is a function of one or more predictors (also called inputs or independent variables) that minimizes the prediction error of one or more target variables (also called outputs). Predictors and targets can be a mix of categorical and scale variables. The topology of RBFNN consists of three layers: input layer, hidden layer and output layer (see Fig.1). This RBFNN proposed here is a special case of multilayer feed forward neural networks, but different in terms of node characteristics and learning algorithms [16].

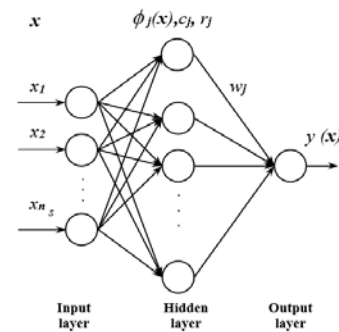


Fig 1. Architecture of radial basis function neural networks.

There is no calculation in input layer nodes. The input layer nodes only pass the input data to the hidden layer. The input layer consist of n_s nodes where input vector $x = (x_1, x_2, \dots, x_{ns})$. The hidden layer consists of n nodes and each hidden node $j = 1, 2, \dots, n$ has a center value c_j . Each hidden layer node performs a nonlinear transformation of the input data onto new space through the radial basis function. The most common choice for the radial basis function is a Gaussian function, given by equation 6:

$$\Phi_j(x) = \exp(-\|x - c_j\|^2 / r_j^2) \quad (6)$$

where: $\|x - c_j\|$ represents the Euclidean distance between input vector (x) and the radial basis function center (c_j). While r_j is the width of radial basis function.

The output layer operation is linear, given by equation 7:

$$y(x) = \sum_j^n w_j \cdot \Phi_j(x) \quad (7)$$

where w_j are the connection weight of hidden layer to output layer and n is number of hidden node.

It is obvious that RBFNN is simply linear combination and to find the easiest solution linear optimization method is used. It converges for a short time and it guaranties convergence to global optimum parameter. Once applying the training process parameters should be defined as follows: *a. Number of nodes in hidden layers, b. the width and center of each radial basis function in each node and c. connecting weight of hidden layer with output layer.*

In order to determine the center and the optimum number of hidden nodes learning algorithm based on orthogonal least square (OLS) is applied [17]. This algorithm function in a forward selection manner selecting the center of a radial basis function one by one in rational way until construction of a suitable network.

3. Discussion results

After application of above two techniques it was possible to get results and to analyse them.

3.1 Multiple regression analysis

The analysis starts from description of variables (see Table 2) which take part in setting up the model following with correlative analysis of them and getting general statistical data (see Table 3) as well as histogram for a significant model (see Fig.2). Some models are important but we have selected like a final model which give us best results in forecasting abilities (see Table 3). The best model of selection is enabled after use of stepwise procedure in SPSS software [11].

Table 2: Descriptive of variables

Productive	Name of variable	Mean	Min	Max	Std.	N
$Y_{Productive}$	Traffic_LOG	2.1030	0.48	4.07	0.9730	39
X_{1D}	Rezidents	47164	1724	204721	45479	39
X_{2D}	ActiveForces	11087	485	58708	11883	39
X_{3D}	Area	298	11	633	176	39
X_{4D}	ActiveBussines	1084	31	10182	1757	39
X_{5D}	Pass.Vehicles	7516	73	48381	8606	39
X_{6D}	Inco. per capita	9482	2242	17772	3132	39
X_{7D}	Density	159	20	531	111	39
X_8	Time	70	5	136	38	39
X_9	Distance	69	10	141	39	39
X_{10}	TripCost	7	1	14	4	39

Table 3: Model summary of statistical parameters

Model Summary ^a					
Model	R	R ²	Adjusted R ²	Std. Error	D.Watson
Productive	0.893	0.797	0.786	0.450	1.676
ANOVA					
Model	SumSquares	df	Mean Square	F	Sig.(p<0.05)
Regression	28.690	2	14.345	70.82	.000
Residual	7.291	36	0.203		
Total	35.982	38			
Coefficients ^a					
	B	Std.Err	t	VIF	Sig.(p<0.05)
Constant	3.167	.168	18.895		.000
Act.ForcesD	3.366E-05	.000	5.479	1.00	.000
Time	-0.021	.002	-10.601	1.000	.000

a. Dependent Variable: ProductiveTrip_LOG

Significant model for productive traffic is given by equation 8:

$$Y_{Productive} = 1468.92 \cdot X_{2D}^{(3.66E-05)} / X_8^{(0.021)} \quad (8)$$

All of the variables are significant at the 5% significance level (95% confidence level) for this model. In other words, (P-value) is <0.05 for all independent variables. It is proved that this is the best for all models because it has the best R², and the lowest ME and

RMSE compared to all other models with the combinations of other variables.

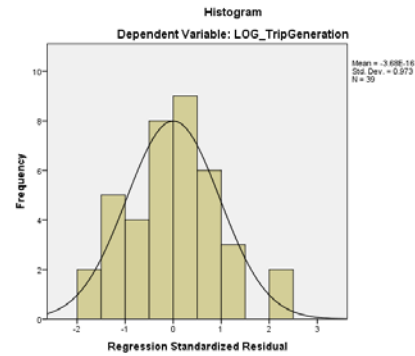


Fig 2. Histogram of regression significant model

The histogram also shows visually that there is approximately normal distribution. Analyzing signs before variables it means that with increase of active forces (X_{2D}) out the region there is increase of traffic while with increase of travel time (X_8) there is decrease of traffic.

3.2 RBFNN analysis

In order to get models through RBFNN we have followed two variants. The first variant: the input variables (13 variables) are in input layer. One hidden layer, and one desired variable (Y) is in output layer with 39 observations are used.

The second variant: only two significant variables which are gained by regression are taken in input layer. One hidden layer, and one desired variable (Y) is in output layer with 39 observations are used. After several attempts it was obvious that the variant with two variables provide much better results of forecasting, respectively in low errors in forecasting. Therefore the further analysis is oriented only to this variant. Data were standardized using the following equation 9:

$$Z = (X - \mu) / \sigma \quad (9)$$

where X is observed value, μ is the mean and σ is the standart deviation. This standartization process yields variable Z with zero mean and unit variance.

For RBFNN analysis, 26 cases (70 %) were assign to the training sample, 9 cases (20%) to the testing sample and 4 cases (10%) to holdout sample. Network information is given in table 4.

Table 4: RBFNN network information

Input Layer	Covariates	1	ActiveForcesD
		2	Time
	Number of Units		2
	Rescaling Method for Covariates		Standardized
Hidden Layer	Number of Units		6 ^a
	Activation Function		Softmax
Output Layer	Dependent Variables	1	TripProduction
	Number of Units		1
	Rescaling Method for Scale		Standardized
	Dependents		Identity
	Activation Function		Sum of Squares
	Error Function		

a. Determined by the testing data criterion: The "best" number of hidden units is the one that yields the smallest error in the testing data.

The RBFNN structure has six units in hidden layers as presented in Fig.3. Also, in table 6 are presented RBFNN model summary. There we can see fewer errors in training than that in testing and holding samples.

Table 5: RBFNN model summary

Training	Sum of Squares Error	0.059
	Relative Error	0.050
	Training Time	0:00:00.02
Testing	Sum of Squares Error	.085 ^a
	Relative Error	.140
Holdout	Relative Error	.427

Dependent Variable: Trip Production

a. The number of hidden units is determined by the testing data criterion: The "best" number of hidden units is the one that yields the smallest error in the testing data.

This is due to the smaller number which is taken into account in testing and holdout samples. However, relative errors in testing and holdout samples are marginal and this has an impact that RBFNN model can be used in the future with high consistency. The architecture and importance of variables of the RBFNN model with two variables in input layer are shown in Fig. 3 and Fig 4.

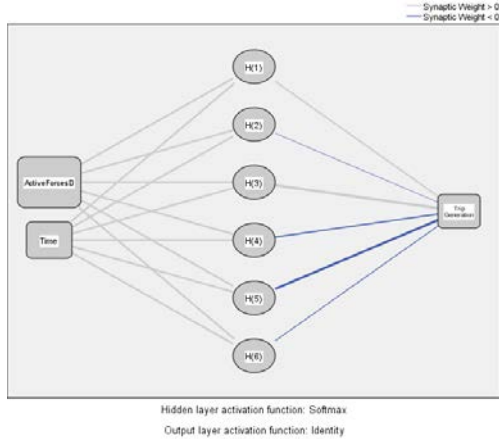


Fig 3. RBFNN Network structure

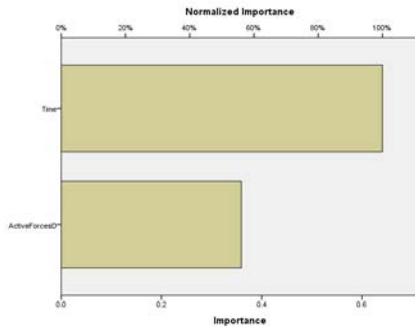


Fig 4. Importance analysis of predictors

3.3 Performance indicators

The most important rule for choosing a forecasting method is its accuracy, or how well they predict matches the actual future value. Here we have used several measures to determine the accuracy of forecasting models and evaluate the performance of models such as: R^2 , ME and RSME.

3.3.1 The coefficient of determination- R^2

Coefficient of determination R^2 can be computed for MRA and RBFNN models using by equation 10:

$$R^2 = \frac{\sum_{i=1}^n [(F_i - \bar{F}) \cdot (A_i - \bar{A})]^2}{\sum_{i=1}^n (F_i - \bar{F})^2 \cdot \sum_{i=1}^n (A_i - \bar{A})^2} \quad (10)$$

where F_i is the i^{th} forecast, A_i is the i^{th} actual values and n is the number of samples. While $\bar{F}$ and $\bar{A}$ are the averages.

Based on this for regression model we have value of $R^2=0.797$, while for RBFNN (RBF 7-2-1) we have calculated separately for training and for testing by expressions below:

$$R_{training}^2 = 1 - \frac{0.059}{39} = 0.998 \quad R_{testing}^2 = 1 - \frac{0.085}{6} = 0.991$$

Variables were rescaled by standardization, it has zero mean and unit variance, and that sum of squares total is equal $n-1$, where n is the sample size.

3.3.2 ME and RSME

These indicators can be calculated separately for two models by equation (11) and (12):

$$ME = \sum_{i=1}^n (F_i - A_i) / n \quad (11)$$

$$RSME = \left[\sum_{i=1}^n (F_i - A_i)^2 / n \right]^{1/2} \quad (12)$$

Table 6: Summary of indicators of R^2 , ME and RSME

Model	R^2	ME	RSME
Regression model	0.797	-146	1778
RBFNN model	0.998	-10	241

Comparing results of Table 6 show that RBFNN model performs much better than ordinary regression in terms of performance indicators explained by the models.

4. Conclusion

In this paper some models are developed but only two of them are selected which is (MRA) and (RBFNN) to get results in traffic production in Anamorava region. The results of those models have been compared to see differences and advantages provided by each of them in forecasting, respectively in finding out which of them provide smaller errors in forecasting. After verification of indicators such as R^2 , ME and RSME by performance analysis we came to conclusion that RBFNN model provide better performance and as such can be fininally used for traffic production forecasting in this region.

5. References

- [1] Elkafoury A. et al. Develop Trip Generation model for Alexandria City-Egypt. Journal of Fluids, Heat and Mass Transfer, Mechanical and Civil Engineering. ISBN:978-1-61804-358-0.
- [2] Arliansyah J. And Haronti Y.: Trip attraction model using radial basis function neural networks. The 5th International Conference of Euro Asia Civil Engineering Forum (EACEF-5). Elsevier & Procedia Engineering, 2015.
- [3] Agency Statistics of Kosovo. General Statistics of Kosovo. Prishtine, 2016.
- [4] Regional Development Strategy for the Economic Region East. Implemented by RDA. Prishtina, 2010.
- [5] Ministry of Infrastructure. Sectorial Strategy of Multimodal Transport 2015-2025 and Action Plan. Prishtina, 2015.
- [6] Ortuzar J.D, Williamson L.G., Third Edition. Modelling Transport.
- [7] Fricker J.D, Saha S.K., 1987. Final Report. Traffic Volume Forecasting Methods for Rural State Highways. Joint Highway Research Project FHWA/IN/JHRP-86/20.
- [8] Semeida A.M., 2014. Derivation of Travel Demand Forecasting Models for Low Population Areas: The case of Port Said Governorate, North East Egypt. Journal of Traffic and Transportation Engineering (English Edition). 1(3):196-2008,
- [9] Varagouli E.G, Simos T.E, Xeidakis G.S., 2005. Fitting a Multiple Regression Line to Travel Demand Forecasting: the Case of Prefecture of Xanthi, Northern Greece. Mathematical and Computer Modelling, 42 (7/8):817-836.
- [10] Navidi W., Statistics for Engineers and Scientists. McGrawHill-Higher Education. ISBN-13:978-0-07-255160-0 and ISBN-10:0-07-255160-7.
- [11] Kalayaci S., 2014.SPSS in Practice. Statistical Techniques with Many Variables. Six Edition.
- [12] Anderson D.R, Sweeney D.J, Williams Th.A., Statistics for Business and Economy. Second piece. Translated in Albanian by published company "UET Press. Tirana.
- [13] Saha K.Sunil and Fricker J.D.: The development of a procedure to forecast traffic volumes on urban segments of the state and interstate highway systems., Final report FHWA/IN/HJHP-90/11, Joint Highway Research Project. School of Civil Engineering, Purdue University, 1990.
- [14] Cicak M.: Modeliranje u zeleznickom saobracaju. Saobracajni Fakultet-Univerziteta u (Book in Serbian). Beogradu,2003.
- [15] Stamenkovic L.J.: Predvidanje emisije gasovnih zagadjujucih materija na nacionalnom nivou primenom modela zasnovanih na vesticim neuronskim mreza. Doktorska disertacija. Tehnoski-Matalurski Fakultet, Univeritet u Beogradu, 2016.
- [16] Aguilar D.P.: A radial basis neural network for the analysis of transportation data. Graduate thesis. University of South Florida, 2004.
- [17] Chen, S., Cowan, C. F. N. and Grant, P. M., Orthogonal Least Squares Learning Algorithm for Radial Basis Function Networks, IEEE, Transaction on Neural Networks, Vol. 2, No. 2, 302-309, 1991.

APPLICATION OF CAD DESIGN OF TECHNOLOGICAL PROCESSES IN THE FIELD OF MATERIAL SCIENCE

Emil Hr. Yankov¹

Nikolay Tontchev²

Simeon Yonchev

¹"Angel Kanchev" University of Ruse, Bulgaria

²"Todor Kableshtov" Higher School of Transport, Sofia, Bulgaria

Abstract. A review of the existing methods applied to multi-criteria decision aiding has been made as well as the multi-criteria approach to a class of problems in the field of material science has been defined. The multi-criteria decision aiding has been successfully applied to determine appropriate compromise decisions about the examined parameters of a number of technological processes of welding, chemical thermal processing, iron covering, etc. The approach presented determines the values of technological factors satisfying the requirements of users simultaneously to a number of values examined and proposes a solution for the relatively highest thresholds at one and the same time

KEY WORDS. SIMULATION, ANN, MODELING, OPTIMIZATION TECHNOLOGICAL PROCESSES.

1. INTRODUCTION

The modern problems of examining the parameters of new and conventional materials and technological processes are multi-criterial and conflict in principle. This nature of the problems is grounded by the fact that, with there examination, it is necessary to provide a certain set of parameters that have to satisfy users' requirements. The solution sought usually consists in determining those combinations of controlling parameters that provide the set of quality parameters specified. The choice of the assessment system of criteria and their rating according to the degree of significance is a problem difficult to formalize. It does not have unambiguous interpretation inevitably causes subjective decisions.

The problem of multi-criteria decision aiding could be most generally defined as a process with:

- a great number of parameters of the solution with a complex interaction among themselves;
- complex cause-and-consequence relations of the solution parameters and the attributes or aims;
- a set of alternatives, which could be reduced to a limited number and in this case the form of cause-and-consequence has to be used.

Due to that reason, looking for an appropriate model to solve a certain multi-criteria problem, one should define first the type of the situation, which is most suitable for solving the problem. An important element of the information base is the component implementing the method of planning the experiment. The main instrument and means of the modern scientific technologies is modeling as by it one can formulate the multi-criteria problem. The models of the complex objects and phenomena are often integrated including contents-describing and formal mathematical parts.

Hence, the study mainly emphasizes on different indices of quality providing including the following groups of criteria: strength (with static and dynamic loading), stiffness (E-module) and toughness (of the material/article), wear-out resistance and hardness, high temperature resistance, appropriate primary cost, compatibility with environment and the possibility of recycling.

2. ANALYSIS OF EXISTING METHODS

An approach to solving the problem (1) is to find the complete set of effective points on the basis of which the decision maker /DM/ chooses one solution. Such algorithms of linear continuous multi-criteria problems have been developed [1], [2]. They have a complex structure and operate slowly. On the other hand, the number of the effective points could be very big and thus make difficult the choice of a decision by the DM.

Another possible approach is to interact directly with the user and his/her preferences to obtain different compromise decisions. In that case, the DM should have a possibility to assess and compare the different solutions obtained. Independently of the

method used to find out an effective point, this point has to reflect the DM's preferences to a certain extent. That is why in the multi-criteria decision aiding (MCDA) generally there are two stages: the stage of a dialog with the DM and the stage of computing the effective point. They are interactive procedures [3], which comprise great part of the well-known methods of solving a MCDA problem.

The criteria thus formulated are directly connected with high serviceability (functionality) and quality (constructional and operational properties) as well as economic efficiency.

The optimal matching of all these trends defines the efficiency of materials, i.e. their capability to meet the challenges of engineering in the best way on each stage of its development. Thus a set of problems of multi-criteria compromise decision-making could be formulated also by multi-criteria compromise optimization of one and the same class for which to is necessary to build an appropriate modern instrument in the process of study.

According to the information available about the DM's preferences, the methods of solving MCDA problems can be divided into three main groups:

1. when the DM is able to give a complete information about his/her preference;
2. when there is not such information available;
3. when this information is given by the DM in the process of solving the problem.

The criteria thus formulated are directly connected with high serviceability (functionality) and quality (constructional and operational properties) as well as economic efficiency.

The optimal combining of all these trends defines the efficiency of materials. The optimal matching of all these trends defines the efficiency of materials, i.e. their capability to meet the challenges of engineering in the best way on each stage of its development. Thus a set of problems of multi-criteria compromise decision-making could be formulated also by multi-criteria compromise optimization of one and the same class for which to is necessary to build an appropriate modern instrument in the process of study.

With the problems in the field of material science, the DM does not have information about his/her preference and for that reason the methods developed within the first group cannot be used.

The second group of methods is characterized by generating the whole set of effective solutions. The set of effective solutions is presented partially or entirely by the DM. Such methods are: the method of weight coefficients or *P* problem [4],[5],[6], the method of limitations [7],[8]; the method of weighed Chebishev's standard [9]. These methods are able to generate the whole set of effective solutions of the MCDA. However, their disadvantage lies in the big calculation resources necessary for generating and the impossibility

or difficulty of the DM to choose a solution from that set. However, they serve as a base of the interactive methods.

The third group of methods does not require knowledge on the function of preference by the DM. They are the base of the interactive man-computer procedures. The DM interacts with the computer (the algorithm set) on the purpose of clearing and giving additional information about the way of reaching a compromise decision.

The methods consist of three basic steps:

1. Giving the DM's requirements;
2. Finding a compromise solution;
3. Checking if the solution found satisfies the DM.

These methods have been developed most intensively for the past few years and are the base of further studies on the problem of MCDA.

The method of limiting planes [10] is very useful for the peculiarities of the problems in the field of material science. This method can be examined as a variation of the method of the admissible destinations. The methods of this class are unique with the approach, which they use to find the best compromise decision. They reduce the area of criteria iteration reflecting the planes and thus eliminating the stage of looking for a destination. Here precise information about trade-off coefficients is required.

3. APPROACH TO SOLVING MULTI-CRITERIA PROBLEMS IN THE FIELD OF MATERIAL SCIENCE.

The multi-criteria approach [10] proposed is characterized with the peculiarity of defining only one effective point of the whole set, which, according to its nature, turns to be fully sufficient for the different processes examined. That solution is characterized with the peculiarity of the problem class being solved and the solutions are with the highest thresholds of the quality indices examined. Their determination is usually assisted by the nature of the multi-criteria problem defined by the regression models of particular parameters of quality. In the field of material science, the latter require relatively one and the same preferences to all criteria as a whole. The solution presented meets the requirements mentioned and corresponds to the maximal effective point. It is determined after the discretization of the variables with certain exactness and building a transformation containing the lowest value of the criteria examined.

Applying this computation technology, technological solutions important for a number of technologies have been obtained and proved in practice [11]-[14].

The approach has been developed in the form of suitable software [10] that automates the calculations and determines the solutions necessary in an extremely easy way.

Before being visualized, the criteria have been put on a normally distributed scale by finding the discrete extremes and excluding the areas where the function has infinite or indefinite values. The movable limits move along this scale filtrating the visualized multi-dimensional spaces and giving a possibility to focus exactly on the decisions, which the researcher is interested in. The multiple criteria approach is used to visualize the numerical transformation of criteria and this visualization is called a filter. Experiments have been made with geometric mean, arithmetic mean, max and min filters and all decisions found out by these filters are non-dominated. The approach visualizes the symbolic data, transforming it into geometric information that helps to form a real picture of the data. The movable limits are a tool, which is used to focus on some details of the picture, thus finding the decisions looked for. The approach helps the decision-maker to get access to the limits as much as possible from the point of view of criteria. This information aids the participation of the decision-

maker's intuition towards the problem and helps him/her to identify and fulfill the aim intentionally

In previous studies, team members conducted research that is summarized in Fig. 1 - Fig.4.

References.

1. Zeleny, M., "Linear Multiobjective Programming", LNEMS, vol. 95, Springer Verlag, Berlin, (1974).
2. Steuer, R., "Multiple Criteria Optimization: Theory, Computation and Application", John Wiley, N.Y., (1986).
3. Rosinger, E., "Interactive algorithm for multiobjective optimization", Journal of Optimization Theory and Applications, vol. 35, No. 3, (1985).
4. Geoffrion, A. M., "Proper efficiency and the theory of vector maximization", J. of Mathem. Analysis and Appl., vol. 22, No. 3, pp. 618-630, (1968).
5. Geoffrion, A. M., "Strictly concave parametric programming. Part I Basic Theory". Mgmt. Sci. No. 13(5), pp. 244-253, (1966).
6. Geoffrion, A. M., J. S. Dyer, and A. Feinberg, "An Interactive Approach for Multicriteria Optimization with an Application to The Operation of an Academic Department", Management Science, 19, pp. 357-368, (1972).
7. Bacopoulos, A., I. Singer, "On convex vectorial optimization in linear spaces". J. Optimization Theory and Applic. 21, pp. 175-188, (1977).
8. Yu, P. L., "Cone convexity, cone extreme points, and nondominated solutions in decision problems with multiobjectives", Journal of Optimization Theory and Applications, No. 49, pp. 430-468, (1974)
9. Bowman, V., "On the relationship of the Chebishev's norm and efficient frontier of multiple-criteria objectives". In: Thiriez H., S. Ziontis (eds.) Multiple criteria decision making (LNEMS vol. 130), Springer, Berlin, pp. 76-85, (1976).
10. Tontchev, N. T. & D. L. Dimitrovski. (1997) Software Providing of Compromise Optimization of Technology processes, Scientific Collections, Vol.1, Aviation and Spaceship, pp.583-589.
11. Toshkov, V., Tontchev, N., Zumbilev, A. On Some Aspects of Minimizing the Energy Expenses at Nitriding of Steels in Glow-Discharge, Jubilee Scientific Session on 50th anniversary of the Technical University in Sofia, 1995, pp.32-36 /in Bulgarian/.
12. Dragolov D. N. Tontchev, Multi-factor Optimization at Technological Regimes Allowing Maximum Precipitation of Manganese and Nickel in Electrolytic Iron – Manganese – Nickel Coverings, Proceedings of the Maritime Scientific Forum, Varna, Volum 1, 1996, pp. 272-277 /in Bulgarian/.
13. Tontchev, N., Toshkov, V & A. Zyumbilev. Multi-Criteria Approach and Computer System of Defining Properties of Alloys Processed Thermally and Chemically-and-Thermally, Proceedings of AMTECH, 97 Scientific Conference, Gabrovo, 1997, pp. 175-182 /in Bulgarian/.
14. Tontchev, N. & G. Valtchev. Multicriterial Optimization of the Properties of Plasma-Sprayed Coatings, Proceedings of Transcom' 97, University of Zilina, pp. 241-244
15. Dimitrov D., Implementation of Contemporary Technologies in Virtualization and Construction of an Information Cloud of Systems for University Needs in the Field of Transport Education, , Proceedings of International Conference on Application of Information and Communication Technology and Statistics in Economy and Education – ICAICTSEE-2014, UNWE, Sofia, 2014r.
16. T.Razmov T., D. Dimitrov , Laboratory Exercise and Course Design on "Project Management" - Third Edition, Todor Kableshkov University of Technology, 2012.

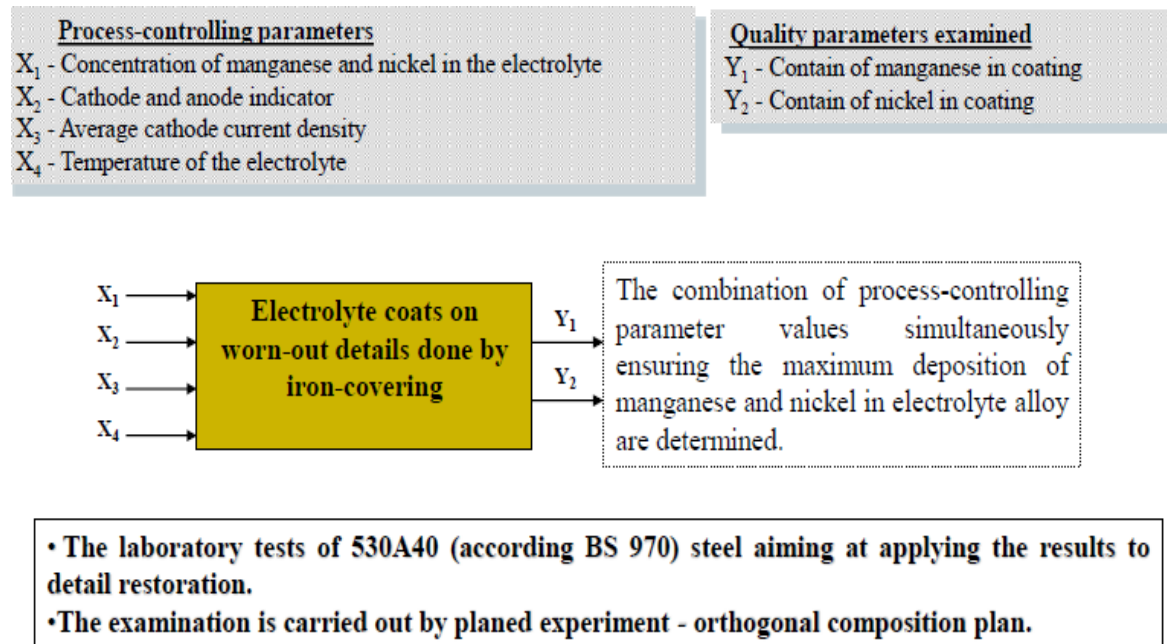


Fig 1. Electrolyte coats on worn-out details done by iron-covering [12]

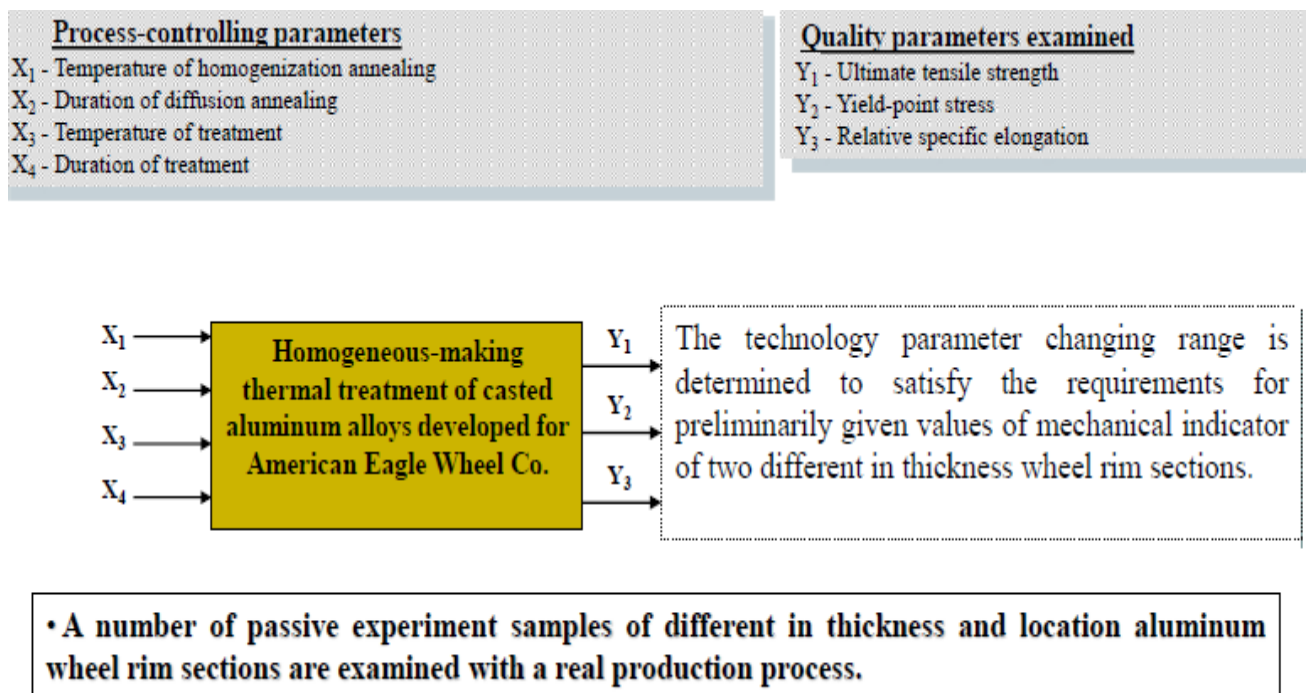


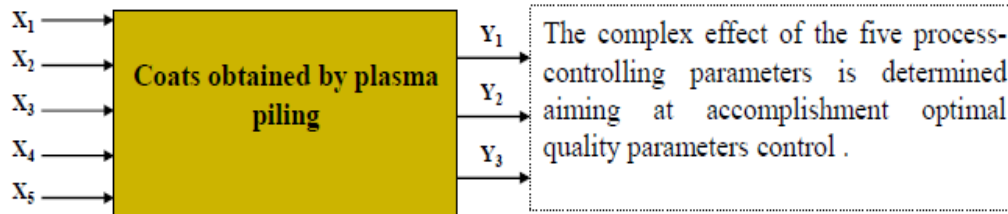
Fig. 2. Homogeneous-making thermal treatment of casted aluminum alloys developed for American Eagle Wheel Co. /Ordered Company Survey/

Process-controlling parameters

X₁ - Consumption of plasma-producing gas
X₂ - Electric arc amperage
X₃ - Distance of piling
X₄ - Displacement speed
X₅ - Powder consumption

Quality parameters examined

Y₁ - Adhesion of the plasma coating
Y₂ - Micro-hardness of the plasma coating
Y₃ - Porosity of coating



- To accomplish the project a planned experiment has been used with Rehshafner's plan.

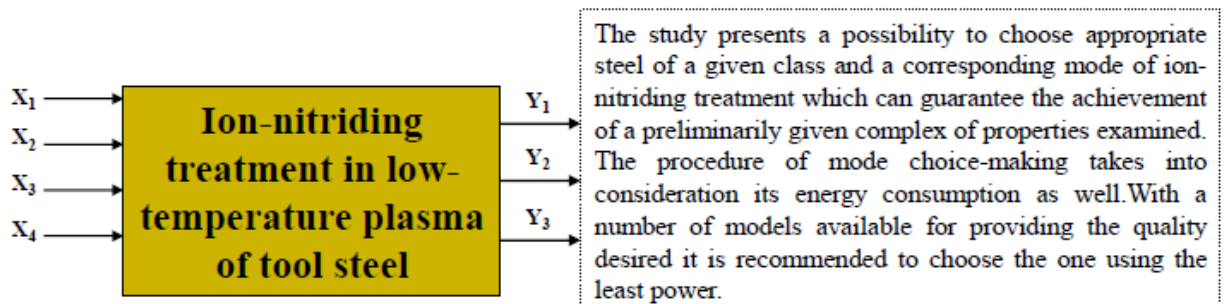
Fig 3. Coats obtained by plasma piling [14]

Process-controlling parameters

X₁ - Temperature ion- nitriding treatment
X₂ - Ammonia pressure
X₃ - Process duration
X₄ - Temperature of tempering

Quality parameters examined

Y₁ - Micro-hardness
Y₂ - Fracture toughness
Y₃ - Relative specific wear resistance



- Laboratory tests of BH11, BH21, BH10 steel types (according BS 4659).
- The examination is carried out by a planned experiment - orthogonal composition plan.

Fig 4. Ion-nitriding treatment in low-temperature plasma of tool steel [11, 13]

SURFACE MORPHOLOGY AND WETTABILITY OF GRADIENT (Ti,Al,V)N/TiO₂ COATING

Nikolova M. PhD.¹

Faculty of Mechanical and Manufacturing Engineering – University of Ruse “A. Kanchev”, Bulgaria¹

mpnikolova@uni-ruse.bg

Abstract: Physical surface properties including surface roughness, topography, morphology, and wettability could influence the implant material behavior, bio-response, bacterial contamination and contact with other bio-active surfaces or fluids. This work investigates micro- and nanoscale roughness parameters and surface morphology of PVD deposited (Ti,Al,V)N/TiO₂ coating using optical microscopy, white light interferometry (WLI), contact profilometer and scanning electron (SEM) microscopy. Results indicated that vacuum oxidized surface possessed medium roughness values, anisotropy in surface texture and irregular morphology. The vacuum oxidation of the nitride maintained the oxide with nano-crystal size and showed pores at the interface between the layers. The effect of prolonged exposure to Ringer-Braun solution droplet on the modified crystalline structure of the oxide was also explained.

Keywords: VACUUM OXIDIZED PVD (TiAlV)N COATING, SEM, WLI, CONTACT PROFILER, WETTABILITY

1. Introduction

The identification, assessment, and quantification of the implant topographic features are essential for ensuring desirable cellular response and successful performance of the implant. In general, the rougher topography shows increased bone apposition in comparison with smooth surfaces (as-machined) that exhibit poor fixation strength [1]. The roughened implant surface serves as adhesion scaffold for the cell facilitating their localization and immobilization. However, compared to the smooth surface, roughened one enhances the accumulation of infectious bacteria [2]. Therefore, surface roughness and texture will determine the healing rate through enabling the bone cell to colonize the implant surface and will contribute to the strength of bone-to-implant contact as well as the surface morphology will exercise influence on bacterial proliferation.

Titanium alloys are commonly employed to manufacture hard tissue replacement, including dental implants, bone plates and artificial hip joints [3]. Many experiments confirmed the feasibility of using TiO₂ thin films as a biocompatible material [4-6]. A mixture of crystalline and amorphous titanium oxide film with a few nanometers thickness is formed naturally in the air. Titanium oxide layers formed at room temperature (e.g. anodically oxidized, sol-gel produced) are often obtained mainly in amorphous form, which can be converted to anatase (300 – 500 °C) or rutile (> 550 °C) by a thermal treatment [7]. The need for crystallization is because the crystal TiO₂ is demonstrated to improve the bioactivity on biomedical implant surfaces [8]. At the same time, a significant temperature-dependent growth of the crystals takes place. The problem that occurs with titanium adhesive joints is that the transformation of amorphous titanium oxide into titanium oxide crystals leads to failure due to the change of oxide volume at the interphase [9]. The amorphous oxides residues could worsen the bonding strength to the crystal substrate. The biological outcomes of anatase crystal architecture are highly significant for implants [10, 11]. Additionally, the micrometer scale surface topography with dimensions comparable to cells possesses the ability to influence cell adhesion, morphology, and contact guidance.

Commonly used surface characterization tools for quantitative analysis are optical microscopy (OM) analysis, white light interferometry (WLI - non-contact optical technique) and scanning electron microscopy (SEM). In this regard, the work reports on surface characteristics of gradient functional (Ti,Al,V)N/TiO₂ coating describe by complementary analysis (OM, WLI and SEM) in order to investigate its topography and morphology. No additional substrate roughening before the modification is applied so as to determine only the surface characteristics of coating and to facilitate the examinations and interpretation of results. The information about the morphological characteristics is used to explain the observed time-related wettability of the modified

surface. The results were post-processed and schematically shown so that they give a more comprehensive set of data.

2. Materials and Methods

Specimens in disk form (Ø20 x 6mm) of commercially pure Ti (cpTi) (Grade 1 in ASTM classification) were prepared by turning and fine-polishing. Thereafter, they were ultrasonically washed with ethanol, acetone, isopropanol and distilled water for 5 min. (TiAlV)N/TiO₂ coatings were deposited on the substrates in a hand-made PVD chamber while the specimens were rotated with a frequency of 0.5 Hz. After loading the specimens, the PVD chamber was evacuated up to a pressure of 1.10^{-4} mbar. A cleaning in glow discharge (substrate bias -400 V) was applied in pure Ar atmosphere at a pressure of $2.5.10^{-2}$ mbar for 60 min. To ensure the coating stress relaxation and necessary adhesion a very thin pure layer from the TiAl5V4 target (at $2.5.10^{-3}$ mbar for 5 min.) was previously applied. Thereafter, the (Ti,Al,V)N film was made by reactive arc deposition in the N₂ atmosphere at 300 °C substrate temperature for a time of 120 min., 120 A arc current (3000 W target power), bias -250 V and $2.5.10^{-3}$ mbar pressure in the working chamber. Directly after deposition, on the (TiAlV)N layer a second TiO₂ film with 0.2-0.3 µm thickness was made by oxidizing, using glow discharge at a negative bias voltage of 400 V in an oxygen atmosphere at a pressure of $2.5.10^{-2}$ mbar for a deposition time of 90 min.

After the PVD patterning and oxidation, the samples were analyzed using an optical microscope (NIKON, Japan) to obtain optical micrographs of the surface of the sample. The images were used to obtain 3D surface plot by Image J software. WLI Photomap 3D (FOGALE Nanotech, France) with sub-nanometer vertical resolution (down to 0.1 nm) at all magnifications, was used to determine roughness parameters for the samples. The two-dimensional surface roughness values of the coatings were measured by MITUTOYO Surftest SJ-201P contact stylus profiler. Scanning electron microscopy (JEOL/EO Version 1.0 JSM-5510) was performed at various magnifications under an acceleration voltage of 10 kV. For wettability studies sessile drop method (CSEM Alpha-Kit CH-2000) was used to measure hydrophilicity by surface contact angle at room temperature after 5 seconds and every 5 minute thereafter with Ringer-Braun solution (8.60 g/L NaCl, 0.30 g/L KCl, 0.33 g/L CaCl₂·2H₂O, pH = 5.7±0.02 at 37°C) droplet. CpTi was used as reference material in order to determine the influence of the oxidation in the (Ti,Al,V)N on the surface hydrophilicity of natural titanium oxide layer and vacuum oxidized one. Before the tests, the surfaces were rinsed with distilled water and dried in air. The droplet of 100 µl volume was pipetted onto the surface using a micro-syringe. It was illuminated with diffuse light in order to obtain an image of the drop with sharp borders. The images were recorded with a camera and the angle between the

baseline of the drop and the tangent at the droplet boundary was measured.

3. Results

Figure 1 shows the software obtained 3D image representing surface characteristics determined by OM. The pseudo-colored height map (Fig. 1) gives a relative view of peaks density without actual roughness values. The measured roughness values by the contact stylus profiler and WLI method are shown in Table 1. Taking into account that the multiphase coating reflects light differently because of the micro-roughened surface, small oxide thickness, underlying (Ti,Al,V)N gold color and its roughness, etc., and the contact method sensitivity limitations, the perceived differences in the average roughness values are identifiable. Although the former factors affect the OM image accuracy, the model surface topography establishes a rough picture of the overall surface morphology.

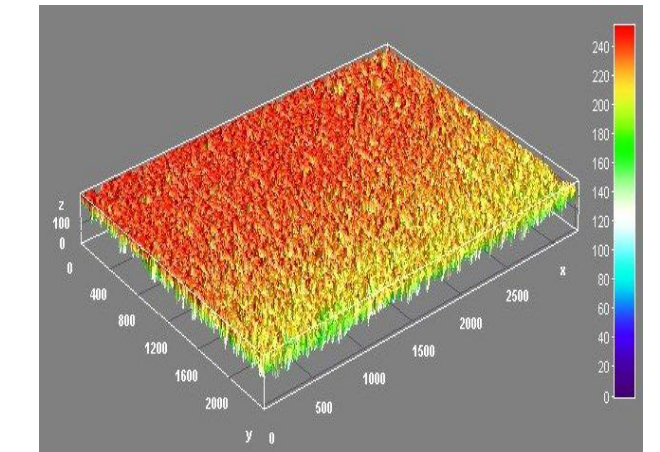


Fig. 1 Optical microscopy 3D model surface (Image J), objective – Nikon x20.

Table 1. Comparison of the average surface roughness values obtained by WLI ($x = 847.51\text{ }\mu\text{m}$, $y = 639.78\text{ }\mu\text{m}$ area) and contact stylus profiler (base line 0.25 mm).

Method	Roughness parameters	R_a , [nm]	R_q , [nm]	R_z , [μm]	R_y , [μm]
Contact stylus profiler	Bare cpTi values	90	95	0.87	0.87
	Coating values	270	370	2.21	2.21
WLI	Roughness parameters	S_a , [nm]	S_q , [nm]	S_p , [μm]	S_v , [μm]
	Coating values	467.45	583.46	2.81	2.43

The WLI measured S_a roughness value for the scanned area of $847.51 \times 639.78\text{ }\mu\text{m}$ is 467.45 nm in contrast to R_a value of 270 nm obtained by the contact profiler. The differences could be attributed to the damageable surface heights during the measurements with the contact profiler. WLI determined that the maximum peak height S_p was equal to 2.81 μm and the maximum valley depth S_v was 2.43 μm . Using WLI analysis, the surface morphological information on the dimensional scale of lateral resolution is as good as 1 μm while the depth resolution reaches down to 1 nm [12]. Despite the lack of contact with the sample and wear of its surface, the lateral pixel sampling was less than the light wavelength and a part of the peaks and sub-micron features were masked which affected the measurements. It is known that WLI can lead to significant errors when applied to measure or image surfaces that contain features that are less than 3 μm in lateral extent and less than 500 nm in height [1] and in this context, including the (Ti,Al,V)N/TiO₂ coating.

SEM is the gold standard in morphology analysis to obtain qualitative descriptions of the surface over multiple length scale and amplitude. In such case, tilting the sample is a useful imaging technique to explore coating morphology and disclose 3D effect.

Typical tilted SEM images providing secondary electron contrast are shown in Fig. 2.

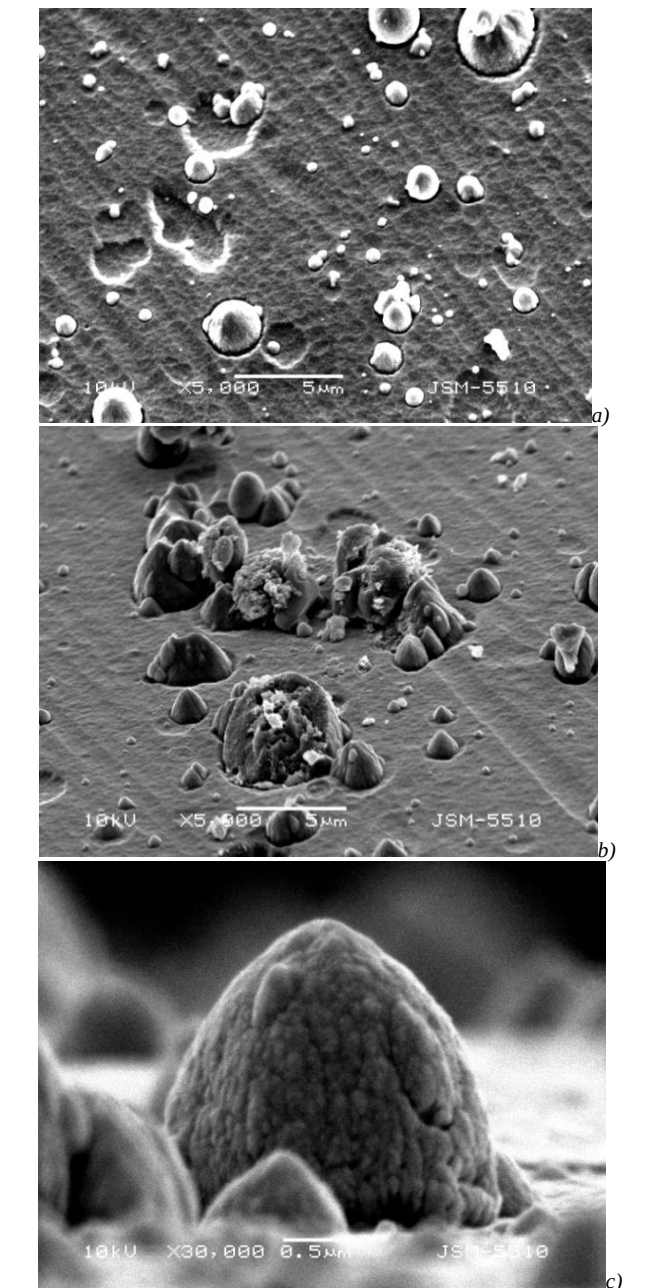


Fig. 2 SEM images (SE contrast); a) top view ($\theta = 10^\circ$); b) tilted topographic image at $\theta = 45^\circ$; c) oxidized droplet of the coating on the surface seen at $\theta = 90^\circ$.

High-resolution SEM revealed clearly the presence of micro- and nanofeatures on the surface of the coating (Fig. 2a). The surface displayed uneven topography with well-defined peaks with semispherical, “vulcanoes”- like shapes and shallow valleys (Fig. 2b). Both peaks and valleys had random distribution on the surface. The higher peaks produced during the Arc deposition of the nitride layer were spread at a distance of about 1 to 30 μm . The finer texture of the flatter surface contained repetitive microwaved morphology with dimensions from 0.5 to 1 μm that corresponded to step growth of the nitride coating. The crystal architecture of the thin nanostructured uppermost TiO₂ on the droplets’ peaks and the flatter nanoscaled surface is demonstrated in Fig. 3c.

The wettability of the surface is important for the adsorption of physiological fluids that take place immediately after the implantation process. The kinetics of contact area evolution of the droplet on the coated surface depending on the interaction time is schematically shown in Fig. 3. It was found out that after 30 min. of emersion, the contact angle value of the coating yielded 18° (Fig.

3a), whereas the smooth titanium surface produced contact angle of 32° (Fig. 3b). Therefore, the Ringer-Braun solution contact angles of the modified substrate showed close to high (but not extremely) hydrophilic properties.

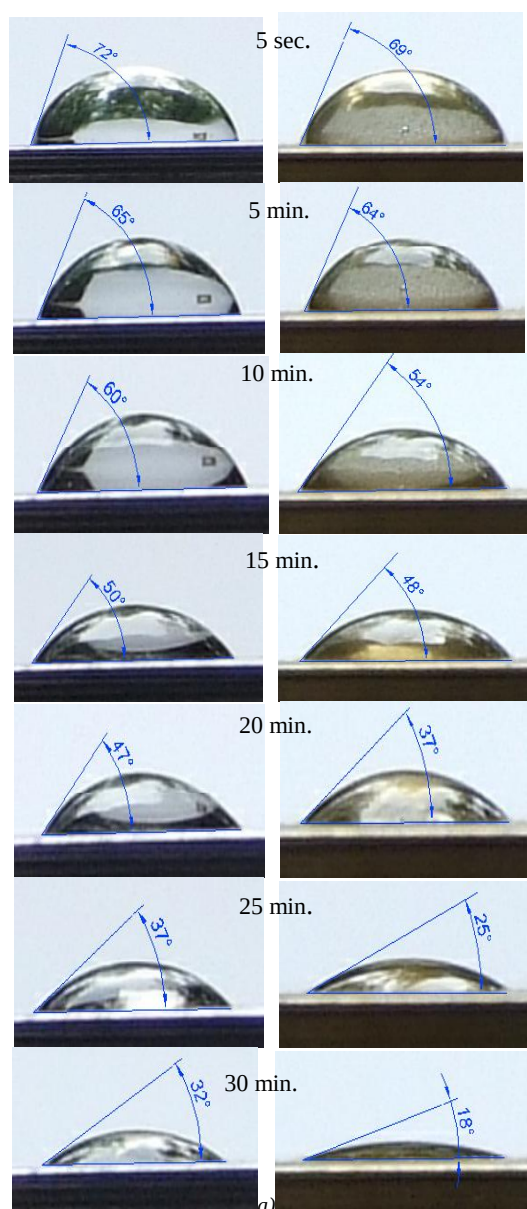


Fig. 3 Measurements of the evolution of contact angle droplet of Ringer-Braun solution with time: a) pristine Ti substrate; b) (Ti,Al,V)N/TiO₂ coated cpTi.

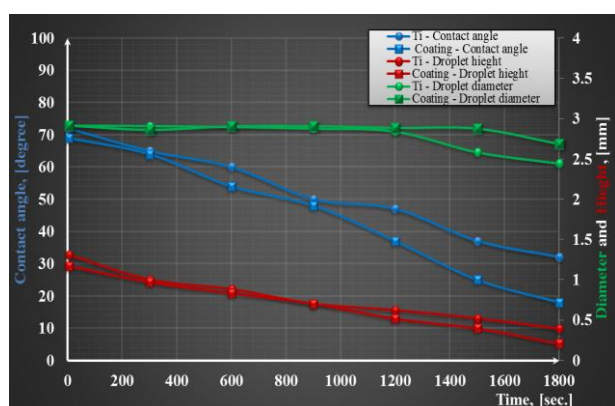


Fig. 4 Comparative measurements of Ringer-Braun solution droplet contact angles, contact diameters D and droplet heights (in mm) with time.

The evolution of the contact angle does not provide information on whether the changes in time were caused by surface morphology

or chemistry or they were related to the kind and way that the molecules were adsorbed. In order to determine if the observed effect is simply due to the surface differences or due to binding strengths and wetting mechanism, the droplets contact diameters and heights were measured. The lines almost parallel to each other were seen for measured values up to 15 min. (Fig. 4), indicating constant droplet diameters and heights of both surfaces. After that moment, the inconsistencies in the measured values increased. The linear slope of the angle and droplet heights decreases with time (20 and 30 minutes) with insignificant change in the droplet diameter, especially for the coated samples.

4. Discussions

The topographic observations indicate that the (Ti,Al,V)N/TiO₂ coating has an anisotropic morphology. As regards the roughness values, S_a (average height) value of 467.45 is more descriptive parameter than R_a due to the latter takes into account a single line profile while S_a parameter determines the whole area observed. Like R_q value, S_q is making sense when the height points are uniformly distributed according to the normal distribution curve [13]. As randomly placed peaks are present on the oxidized coating, the S_q values are not precisely determined but in comparison with a smooth sample ($S_q < 0.1$ nm), the topographic parameter S_q (583.46 nm) of the modified surface is enhanced. There is conflicting work in the literature whether an ordered topography or a disordered topography is superior in soliciting a favorable cellular response and effective protein adsorption [14]. Despite having relatively low values, it is commonly accepted that the moderately rough surfaces (500 nm up to 2 μ m) have shown better results concerning osseointegration.

The SEM analysis clearly reveals the micro- and nanofeatures on the modified surface. On the (Ti,Al,V)N/TiO₂ coating the larger pits sidewalls are smooth with gradually decreasing curvatures and their bottoms are flattened. On the basis of the shallow valleys with small size and form, it could be suggested that the larger depressions are the result of the droplets initial attack and interference with surface and their movements before condensation. Such valley morphology would less entrap and even impede the bacterial rigid cell wall to adhere. Furthermore, considering the crystalline structure of the oxide, seen in Fig. 2c, its crystal architecture would be more beneficial for the decreased bacterial proliferation because Del Curto B et al. [15] discovered that the amorphous TiO₂ promote bacterial attachment. According to Pokrowiecki R. et al. [16], nano-rough titanium plates were much less colonized by bacterial cells than the conventional machined surface.

The wetting behavior differences upon emersion should be considered in conjunction with the differences in the surface structure of the oxide. After pipetting, the molecules and ions on both samples are physically adsorbed to the surface with no systematic orientation (Fig. 3). The Ti-O bond is generally thought to be ionic with negligible covalence. Even in the presence of small quantity of Al, Ti atoms bond stronger to the O than Al [17]. Increasing the time of emersion, due to the hydrophilic interaction surface monolayer of amphiphilic water molecules orients close to the surface in order to compensate the ionic surface polarization charge. On one hand, the increase of surface energy (decrease of the contact angle) of the modified surface can be related to the increase of surface roughness. In contrast, on polished cpTi the naturally formed compact oxide film is discovered to show predominant flat morphology and thickness of 3.17 nm achieved after 1 day of exposure to air [18]. For the machined cpTi Mendonça G. et al. [19] found no evidence of nanofeatures on the surface. In the particular case, the topographical pattern of the surface modification decreases the contact angle compared to the polished cpTi surface even at 5 sec. time. The nanostructured oxide morphology of the coating unequivocally established a nanoscaled roughness (Fig. 3) with an increased number of atoms and, therefore, charge density on the surface. The considerable vertical surface roughness influences not

only its topography but also increases the coating superficial area. Thus, the superficial activity of the real surface area is increased and the quantities of the H-bonds and ions interactions are substantially greater.

However, the slope of the angle decreases with time (20 and 30 minutes) with insignificant change in the droplet diameter (Fig. 4), indicating an increase in adsorbate-surface interactions. Due to the liquid penetration in the modified surface, the effective area wetted by the solution in case of micro- and nano-rough surfaces is larger than the area of the smooth surface. It is likely the liquid to penetrate deeper in the oxidized coating because of the intrinsic polarity of the material. In the bottom side of the oxide, the fine-grained morphology and its uneven structure that contains pores with different sizes are also seen (Fig. 5 b). The reasons for the presence of larger pores are the smaller droplet phases surrounded by the oxide that remained unstuck at the nitride surface (Fig. 5a).

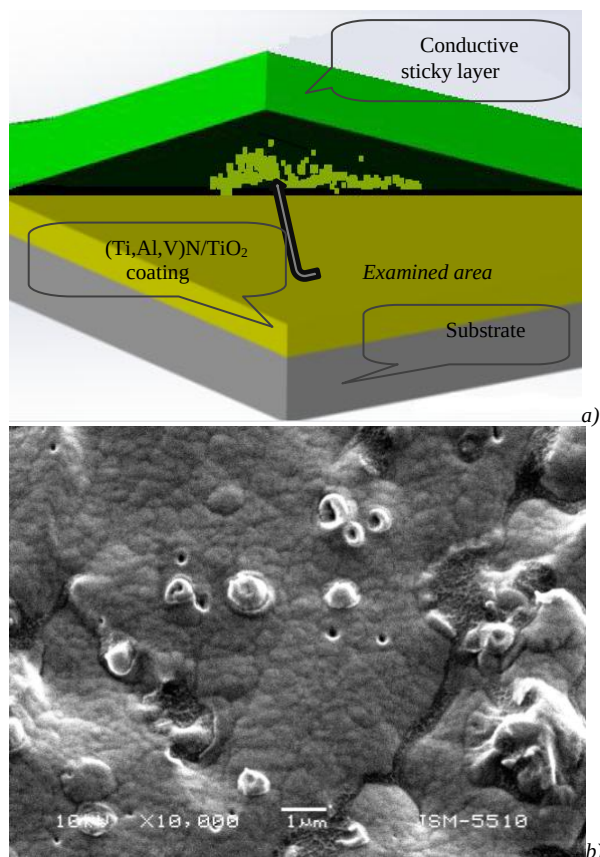


Fig. 5 Oxide characteristics: a) scheme of the surface sampling for examining the bottom area of the oxide; b) SEM images (SE mode) of surface oxide structure at the bottom side.

The other reason for the small covered pores presence at the oxide-nitride interference suggests not only the explanation of oxide-solution interaction but the mechanism of (Ti,Al,V)N oxidation. It follows that near to the surface the nitride undergoes complete phase transformation during the oxidation procedure. Underneath the TiO_2 area, the low temperature of the glow discharge during vacuum oxidation does not provide high mobility of oxygen species for complete phase segregation. Then, below the surface oxide, a complex titanium oxy-nitride nanostructure is reasonable to be expected. In addition to the interstitial atom positioning, lateral fluxes of oxygen through already existing voids, defects and/or strained parts in the small grains could be estimated. The highly reactive oxygen atoms are likely to occupy the nitrogen position in the fcc lattice of the nitride. Nitrogen atoms recombination during oxidation process should be considered as the cause for the pore presence at the oxide-nitride interface. The precipitation of molecular nitrogen (N_2) would be favored at grain boundaries of the nitride sublayer. The nitrogen depletion provokes augmented titanium oxidation rate in depth. The residual N atoms occupied O-atoms sides in the TiO_2 to form Ti-N bonds. As the

vacancy mechanism is known to be more effective than simply expanding the lattice volume, many processes including adsorption, diffusion, incorporation, chemical reactions etc., impact the kinetic coefficients of the processes. The charge compensation is likely to experience downward-pointing electrical gradient near to the surface and below it (in the pores) because of the potential effect inside the micro- and nanopores. Schematic representation of the process is shown in Fig. 7.

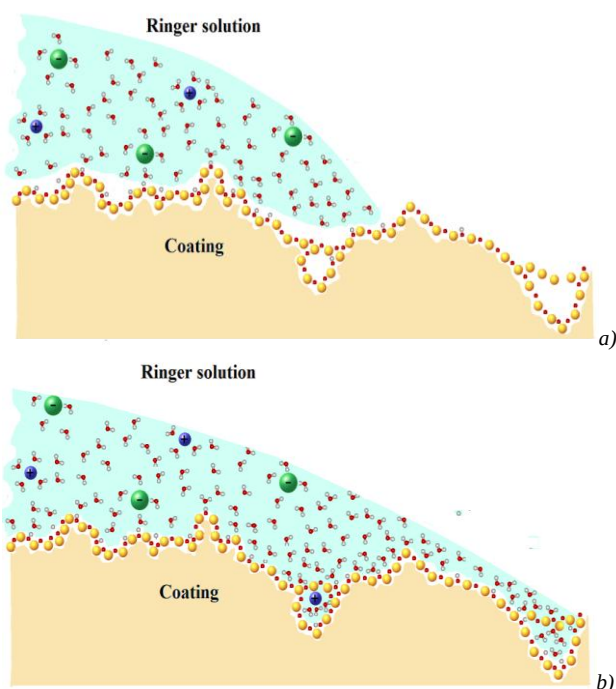


Fig. 6 Scheme of time-dependent interaction of the coated sample with Ringer-Braun solution droplet: a) initial contact; b) evolution of the adsorbate-surface interactions in time.

This electrostatic field is also caused by the enhanced compressive strain that follows the nitride-oxide transformation near to the surface. This is because in crystalline TiO_2 the Ti atoms bond with six oxygen atoms that form an octahedral structure and O atoms prefer three titanium atoms as neighbors. As the crystal ionic radii of Ti^{4+} is 74.5 pm and the O^{2-} is 126 pm (in contrast to Ti^{3+} - 81 pm and N^{3-} - 134 pm), the lattice parameter of TiO_2 decreases with increasing the oxygen content. Because the oxygen concentration decreases in depth (not shown), the nitride-oxide transformation leads to compressive stress state development near to the surface. The local volume decrease within nitride – oxide phase transformation accompanies strains that contribute to the geometry and strength of adsorbate-surface interactions and capillary phenomenon. For that reason, the relative change in the droplet height with the increase of time substantially decreases for the coated sample (Fig. 7) while the drop diameter stays merely unchanged.

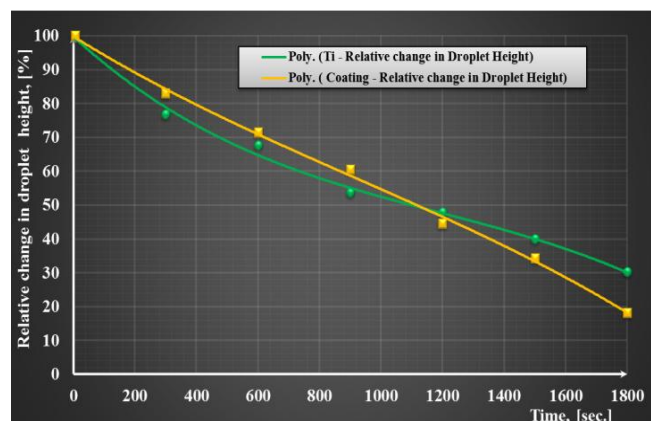


Fig. 7 Relative change in the Ringer-Braun droplet height in time.

The Ringer-Braun solution paths for penetration into the interfacial areas via diffusion processes or capillary attraction are tightened at the surface because of the compressive stresses in the coating. The discrepancy in the contact angle values increases with time indicating that the molecules and/or ions from the solution access the coating in depth via pinholes in the TiO₂ layer that are not initially accessible. The porous surface can absorb parts of the solution and because of that, the drop floats in. In this way, the adsorbate-surface interactions increase their strength.

5. Conclusions

In this study biomimetic approach of micro- and nano-metric modification by means of a deposition of a nitride PVD coating and its vacuum oxidizing is used. Complementary topography and morphology analysis in addition to statistical roughness description is performed to obtain a definitive characterization of the (Ti,Al,V)N/TiO₂ surface that is essential to understand different biological effects. The numerous features seen in SEM images show a qualitative difference between OM representation and more comprehensive view at two length scale. The composite film tended to be irregularly rough. The irregular features were random groups of “volcanoes” with different size (from tens of nanometers to several micrometers) and flat valleys with various sizes. The peak-to-peak distance was of the order of about one to five micrometers. The surface morphology was regulated by the physical processes of condensation, crystallographic pre-determined growth, and specific nitride oxidation. The micro- and nano-features of the underlying film and the oxide thickness determine the structure of the overlying oxide. By studying the changes in the drop contact angle it could be seen that the increased wettability compared to the polished cpTi surface was due to a combination of the surface roughness, oxidative treatment, nanocrystal oxide characteristics, coating pattern, and porosity. It is well known that the increased wettability is highly recommended for implant surfaces because the hydrophilic surface has a beneficial impact on the proteins conformation and their folding activity. Simultaneously, the permission of solution along the sidewall down to the substrate could trigger corrosion processes in the implant material. Then the most fundamental question - which surface chemistry or morphology is more important, remains still unanswered.

Acknowledgements

The financial support of this work was provided by the National Science Fund of Ministry of Education and Science, Bulgaria, under Grant project “Gradient functional nano-coatings produced by vacuum technologies for biomedical applications” with number D№ 07/3 (2016).

The author would like to thank D-r Marius Bazu and Phys. Raluca Gavrilă from IMT-Bucharest for their assistance with using the institute facilities (WLI) as well as D-r Emil Yankov and Assoc. prof. Danko Tonev for their support in some measurements.

LITERATURE

- Sosale G., Measurement and Analysis of Surface Topography over Multiple Length Scales: Application to Titanium Bone Implants, Thesis for Master degree of Engineering, McGill University Montreal, Canada 2007;
- Harris L.G, R.G. Richards, Staphylococci and implant surfaces: a review. *Injury* 37, 2006, (Suppl. 2);
- López-Huerta F., B. Cervantes, Biocompatibility and Surface Properties of TiO₂ Thin Films Deposited by DC Magnetron Sputtering *Materials* 7, 2014, 4105-4117; doi:10.3390/ma7064105;
- Niinomi, M. Biologically and mechanically biocompatible titanium alloys. *Mater. Trans.* 49, 2008, 2170–2178;
- Elias, C. N., J. H. C. Lima, R. Valiev, M. A. Meyers, Biomedical applications of titanium and its alloys. *J. Miner. Met. Mater. Soc.* 2008, 60, 46–49
- Okazaki, Y. On the effects of hot forging and hot rolling on the microstructural development and mechanical response of a biocompatible Ti alloy. *Materials* 2012, 5, 1439–11461
- Killian M. S., Organic Modification of TiO₂ and other Metal Oxides with SAMs and Proteins - a Surface Analytical Investigation, Dissertation, Friedrich-Alexander-Universität Erlangen-Nürnberg, 2013
- Lin C.C., H.C. Cheng, C.F. Huang, C.T. Lin, S.Y. Lee, C.S. Chen, K.L. Ou, *J. Appl. Phys.* 44 (12) (2005) 8590- 8598
- Shirazi S. N., Wet chemical surface modifications of Titanium and Ti6Al4V alloy and their effect on the hydrothermal aging mechanisms and adhesion properties Dissertation, Bremen, 2010
- He J., W. Zhou, X. Zhou, X. Zhong, X. Zhang, P., Wan, B. Zhu, W. Chen, The anatase phase of nanotopography titania plays an important role on osteoblast cell morphology and proliferation. *J. Mater. Sci. Mater. Med.* 19, 2008, 3465–3472;
- Sollazzo V., F. Pezzetti, A. Scarano, A. Piattelli, L. Massari, G. Brunelli, F. Carinci, Anatase coating improves implant osseointegration in vivo. *J. Craniofac. Surg.* 18, 2007, 806–810;
- Albrektsson T., L. Sennerby, A. Wennerberg, State of the art of oral implants. *Periodontology* 2000, 2008, 47, pp.15-26;
- Raposo M., Q. Ferreira, P.A. Ribeiro, A Guide for Atomic Force Microscopy Analysis of Soft Condensed Matter, ©FORMATEX 2007, Modern Research and Educational Topics in Microscopy. A. Méndez-Vilas and J. Díaz (Eds.);
- Le, X., G.E.J. Poinern, N. Ali, C.M. Berry, D. Fawcett, Engineering a Biocompatible Scaffold with Either Micrometre or Nanometre Scale Surface Topography for Promoting Protein Adsorption and Cellular Response, *International Journal of Biomaterials*, 2013, pp. 1-16., <http://dx.doi.org/10.1155/2013/782549>;
- Del Curto B., M.F. Brunella, C. Giordano, M. P. Pedferri, V. Valtulina, L., Visai, A. Cigada, Decreased bacterial adhesion to surface-treated titanium. *Int J Artif Organs* 2005, 28 (7): 718-30;
- Pokrowiecki R., B. Szaraniec, J. Chłopek, M. Zaleska, Recent trends in surface modification of the titanium biomaterials used for endosseous dental implants, *Engineering of Biomaterials* 124 (2014) 2-10;
- Magnuson M., M. Mattesini, S. Li, C. Höglund, M. Beckers, L. Hultman, O. Eriksson, Bonding mechanism in the nitrides Ti₂AlN and TiN: an experimental and theoretical investigation, *Physical Review B* 76, 2007, 195127
- Harmankaya N., Titanium Oxide and Bone Anchorage Role of the Complement System, and Delivery of Osteoporosis Drugs from Mesoporous TiO₂, *Sahlgrenska Academy at University of Gothenburg*, 2013;
- Mendonça G., D. Baccelli, S. Mendonça, L. Gustavo, P. Simões, A. L. Araújo, E. R. Leite, A. L. Golin, F. J L Aragão, L. F. Cooper, Nanostructured implant surface effect on osteoblast gene expression and bone-to-implant contact in vivo *Materials Science and Engineering C* 31 (8), 2011, 1809–1818;