

INTERNATIONAL SCIENTIFIC JOURNAL



SCIENCE. BUSINESS. SOCIETY.

YEAR 1, ISSUE 6/2016

ISSN PRINT 2367-8380

ISSN WEB 2534-8485

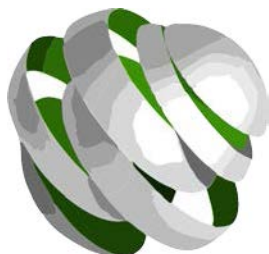
PUBLISHERS:



SCIENTIFIC TECHNICAL UNION OF MECHANICAL ENGINEERING

108 RAKOVSKI STR., SOFIA 1000, BULGARIA

NATIONAL SOCIETY "INDUSTRIAL & NATIONAL SECURITY"



INTERNATIONAL SCIENTIFIC JOURNAL
SCIENCE. BUSINESS. SOCIETY

PUBLISHER:

**SCIENTIFIC TECHNICAL UNION OF MECHANICAL ENGINEERING
NATIONAL SOCIETY "INDUSTRIAL & NATIONAL SECURITY"**

108, Rakovski Str., 1000 Sofia, Bulgaria
tel. (+359 2) 987 72 90,
tel./fax (+359 2) 986 22 40,
office@stumejournals.com

ISSN PRINT: 2367-8380

ISSN WEB: 2534-8485

YEAR I, ISSUE 6 / 2016

EDITORIAL BOARD

CHIEF EDITOR

Prof. Dimitar Yonchev, Bulgaria

RESPONSIBLE SECRETARY:

Assoc. Prof. Hristo Karamishev, Bulgaria

MEMBERS:

Prof. Detlef Redlich, Germany	Prof. Sabina Sestic, Bosnia and Herzegovina
Prof. Ernest Nazarian, Armenia	Prof. Senol Yelmaz, Turkey
Prof. Garo Mardirosian, Bulgaria	Prof. Shaban Buza, Kosovo
Prof. Georgi Bahchevanov, Bulgaria	Assoc. Prof. Shuhrat Fayzimatov, Uzbekistan
Assoc. Prof. Georgi Pandev, Bulgaria	Prof. Sveto Cvetkovski, Macedonia
Prof. Iurii Bazhal, Ukraine	Prof. Teymuraz Kochadze, Georgia
Prof. Lyubomir Lazov, Latvia	Assoc. Prof. Veselin Bosakov, Bulgaria
Prof. Ognyan Andreev, Bulgaria	Prof. Vladimir Semenov, Russia
Prof. Olga Kuznetsova, Russia	Prof. Yuriy Kuznetsov, Ukraine
Assoc. Prof. Pencho Stoychev, Bulgaria	Prof. Zhaken Kuanyshbaev, Kazakhstan

CONTENTS

SCIENCE

ON REGULAR PARALLELISMS OF PG(3,5) WITH AUTOMORPHISMS OF ORDER 5 Dr. Zhelezova S.	3
MOLECULAR MODELING AND CREATING 3D MODELS OF CHEMICAL COMPOUNDS IN BLENDER SOFTWARE USING THE RESOURCES OF CHEMSPIDER AND OPEN BABEL Phd Tihomir Dovramadjiev	6
MOLECULAR SIMILARITY IN THE FRAMEWORK OF A BIOISOSTERISM STUDY Desislava Ivanova	8
SOFTWARE DESIGN M.Sc. Ivanova Milka	11

BUSINESS

MATHEMATICS INDUSTRY ECONOMY – MICRO-FOUNDRY Bushev St. PhD. assoc. prof. eng.	15
THE PROBLEM OF OVERLAPPING PROJECT ACTIVITIES WITH INTERDEPENDENCY Prof. Gurevich G., Prof. Keren B., Prof. Laslo Z.	18
SUMMARY OF INNOVATION MODELS ON A COMPANY LEVEL – CREATING A FRAMEWORK FOR AN INNOVATION MODEL THAT WILL INCREASE A COMPANY’S INNOVATION ACTIVITY M.Sc. Stefanovska Ceravolo LJ., Prof. PhD. Polenakovikj R., Prof. PhD Dzidrov M.	22
TOP INNOVATION IN MANAGEMENT OF AGRICULTURAL ACTIVITIES (EFFECTIVE BIOLOGICAL AGRICULTURE UNDER IRRIGATION AND PROTECTING THE ENVIRONMENT) Prof. Dr. Christov I., Ph.D. & D.Sc.	26

SOCIETY

AN APPROACH TOWARDS PLANNING OF ELECTRIC VEHICLES CHARGING INFRASTRUCTURE BASED ON VEHICLE AND TRANSPORT STRUCTURE M-r Stevan Kjosevski, dipl. mech. engineer, PhD student, Prof. d-r Atanas Kochov, dipl. mech. Engineer, Doc. d-r Aleksandar Kostikj, dipl. mech. Engineer	30
PRESERVATION OF POLLUTION OF DANUBE RIVER WATERS Ass.Professor PhD Kremena Bozhidarova Rayanova	35
INTERNATIONAL LEGAL MEASURES FOR AVOIDANCE OF SEA POLLUTION WITH PETROL Chief Asst. PhD Vanya Velichkova Panteleeva	37
IDEOMOTORIC TRAINING AS A TOOL FOR PROFESSIONAL RELIABILITY IMPROVEMENT AMONG POLICE OFFICERS As. prof., dr. psych. Kalinnikova, L., ma. psych. Zavodilov, A.	40

ON REGULAR PARALLELISMS OF $PG(3,5)$ WITH AUTOMORPHISMS OF ORDER 5

ОТНОСНО РЕГУЛЯРНИТЕ ПАРАЛЕЛИЗМИ НА $PG(3,5)$ С АВТОМОРФИЗМИ ОТ РЕД 5

Dr. Zhelezova S.,¹

Institute of Mathematics and Informatics, Bulgarian Academy of Sciences, Bulgaria

e-mail: stela@math.bas.bg

Abstract: A spread is a set of lines of $PG(n,q)$, which partition the point set. A parallelism is a partition of the set of lines by spreads. A regulus of $PG(3,q)$ is a set R of $q+1$ mutually skew lines such that any line intersecting three elements of R intersects all elements of R . A spread S of $PG(3,q)$ is regular if for every three distinct elements of S , the unique regulus determined by them is a subset of S . A parallelism is regular if all its spreads are regular.

Regular parallelisms in $PG(3,q)$ are known for any $q \equiv 2 \pmod{3}$ due to T. Penttila and B. Williams, 1998. In $PG(3,5)$ these families of regular parallelisms are presented by two regular parallelisms with automorphisms of order 31 obtained early by A. Prince. Whether these are all regular parallelisms in $PG(3,5)$ is an open question.

There are four relevant groups of order 5 and in the present paper it is established that the regular parallelisms of $PG(3,5)$ cannot possess any automorphism of order 5.

Keywords: PARALLELISM, AUTOMORPHISM, REGULARITY, COMBINATORIAL DESIGN

1. Introduction

Parallelisms are used in constructions of constant dimension error-correcting codes that contain lifted maximum rank distance codes. They are closely related to resolutions of Steiner systems and therefore they can be used for cryptographic anonymous $(2,q+1)$ -threshold schemes.

Regular parallelisms are connected to translation planes. Lunardon [9] and also Walker [17] established that every regular parallelism in $PG(3,q)$ may be used to construct a spread in $PG(7,q)$, and hence a translation plane of order q^4 with kernel $GF(q)$ that admit $SL(2,q)$ as a subgroup of their automorphism group.

For the basic concepts and notations concerning spreads and parallelisms of projective spaces, refer, for instance, to [6], [8] or [15].

A **spread** in $PG(n,q)$ is a set of lines which partition the point set. A **parallelism** (line parallelisms) is a partition of the set of lines by spreads. There can be line spreads and parallelisms if n is odd.

Two parallelisms are **isomorphic** if there exists an automorphism of the projective space which maps each spread of the first parallelism to a spread of the second one.

A subgroup of the automorphism group of the projective space which maps each spread of the parallelism to a spread of the same parallelism is called **automorphism group** of the parallelism.

There are some general constructions of parallelisms: in $PG(n,2)$ by Zaitsev et al. [19] and independently by Baker [1], and in $PG(2n-1,q)$ by Beutelspacher [3]. Several constructions are known in $PG(3,q)$ due to Denniston [4], Johnson [8], Penttila and Williams [10].

Computer aided classifications of parallelisms are also available. Stinson and Vanstone classified parallelisms of $PG(5,2)$ with a full automorphism group of order 155 [14] and Sarmiento with a point-transitive cyclic group of order 63 [13]. Topalova and Zhelezova classified parallelisms of $PG(3,4)$ with automorphisms of order 5 [16]. Recently all parallelisms of $PG(3,3)$ were classified by Betten [2].

A **regulus** of $PG(3,q)$ is a set R of $q+1$ mutually skew lines such that any line intersecting three elements of R intersects all elements of R .

A spread S of $PG(3,q)$ is **regular** if for every three distinct elements of S , the unique regulus determined by them is a subset of S . A parallelism is regular if all its spreads are regular.

Parallelisms of $PG(3,2)$ are regular. Denniston [5] showed two regular parallelisms in $PG(3,8)$. Among the constructed by Prince [11] parallelisms of $PG(3,5)$ with automorphisms of order 31 there are two regular ones. Next Penttila and Williams constructed two families of regular cyclic parallelisms of $PG(3,q)$ for any $q \equiv 2 \pmod{3}$ [10]. All presently known examples of regular parallelisms are among them and the existence of other regular parallelisms is an open question.

2. Construction and results

To construct $PG(3,5)$ we use the 4-dimensional vector space over $GF(5)$. The points of $PG(3,5)$ are then all 4-dimensional vectors (v_1, v_2, v_3, v_4) over $GF(5)$ such that if $v_k = 0$ for all $k > i$ then $v_i = 1$. We sort these 156 vectors in ascending lexicographic order and then assign them numbers such that $(1,0,0,0)$ is number 1, and $(4,4,4,1)$ is number 156.

There are 806 lines in $PG(3,5)$. We sort them in ascending lexicographic order defined on the numbers of the points they contain and assign to each line a number according to this order. The first line contains points $\{1,2,3,4,5,6\}$ and the last one (806) – $\{31,56,75,94,113,132\}$.

A spread has 26 lines which partition the point set and a parallelism has 31 spreads.

The main steps of the used method for constructing regular parallelisms with the chosen automorphism group are:

- construction of all regular spreads;
- test the regular spreads if they are invariant under the chosen automorphism group or all its lines are from different orbits under the chosen automorphism group;
- combine the obtained orbit leaders to form a parallelism.

We are interested in regular parallelisms so we begin with the construction of regular spreads. We use backtrack search on the lines [20]. A regular spread of $PG(3,5)$ contains:

$$\binom{q^2+1}{3} / \binom{q+1}{3} = 130 \text{ reguli.}$$

For each of the 31 lines containing the first point 5000 regular spreads are obtained. This number can be verified by:

$$\frac{1}{2}q^4 \cdot (q-1)^2 \quad [18].$$

Denote by G the full automorphism group of $PG(3,5)$. $G \cong P\Gamma L(4,5)$ and it is of order $2^9 \cdot 3^2 \cdot 5^6 \cdot 13 \cdot 31$. The Sylow 5-subgroups of G have order 5^6 . We use GAP [7] to find an arbitrary Sylow 5-subgroup $G_{5,6}$. It has 6 subgroups of order 5 which are in four conjugacy classes. Any subgroup of G of order 5 is in one of these four conjugacy classes.

With respect to the group action a spread can be of two types:

- fixed – contains the whole orbit of any of its lines;
- not fixed – its lines are from different orbits of one and the same length.

To form a fixed spread some fixed lines are needed together with some of the orbits consisting of skew lines. If a spread is not fixed, we choose for it lines with orbits of one and the same length. Therefore, we already know the other spreads of its orbit. We call the first one *orbit leader* (a fixed spread is also an orbit leader). To obtain a parallelism we need to obtain only the orbit leaders.

We take an arbitrary subgroup of order 5 from each conjugacy class, namely we consider the following four subgroups:

- subgroup G_{5_1} which fixes 31 points and 56 lines and partitions the lines in 150 orbits;
- subgroup G_{5_2} which fixes 6 points and 31 lines and partitions the lines in 155 orbits;
- subgroup G_{5_3} which fixes 6 points and 6 lines and partitions the lines in 160 orbits;
- subgroup G_{5_4} which fixes a point and a line and partitions the lines in 161 orbits.

Each of these subgroups has at least one fixed line, therefore a resolution has to contain some fixed spreads and the remaining spreads have to be in orbits of length 5.

There aren't orbits consisting of skew lines under the action of subgroup G_{5_1} , so a fixed spread cannot be formed. Therefore a resolution with G_{5_1} doesn't exist.

The subgroup G_{5_2} fixes 31 lines and 30 of the line orbits are with skew lines. The parallelisms invariant under G_{5_2} have:

- one fixed spread containing a fixed line and 5 orbits with skew lines;
- five fixed spreads containing six fixed lines and 4 orbits with skew lines;
- five orbits of five spreads each.

There are 250 regular spreads with a fixed line but noone with six fixed lines, hence a regular resolution with G_{5_2} doesn't exist.

The subgroup G_{5_3} fixes the first 6 lines in our lexicographic order, which cover the first 31 points. They share a point (point 1) so each of them has to be in different spread. The smallest point which is in a orbit with skew lines is point 12. Each line in $PG(3,5)$ is incident with six points, so to cover all points until point 12 at least two fixed lines are needed. That is why a resolution with G_{5_3} doesn't exist.

The subgroup G_{5_4} fixes a line and 100 of the line orbits are with skew lines. The parallelisms invariant under G_{5_4} have:

- one fixed spread containing a fixed line and 5 orbits with skew lines;
- six orbits of five spreads each.

There are 33441 regular spreads with orbit of length 5 but noone with a fixed line, hence a regular resolution with G_{5_4} doesn't exist.

3. Conclusion

We compute the necessary groups and its conjugacy classes using GAP. Our C++ programmes performing the computer computations are based on the exhaustive backtrack search techniques.

Since software mistakes are always possible, we obtain the same number of regular spreads in $PG(3,4)$ as in [12]. To test our software we construct two regular parallelisms of $PG(3,2)$.

As a result of our investigation we can conclude that two of the subgroups of order 5 (G_{5_1} and G_{5_3}) cannot produce any parallelism in $PG(3,5)$ while the other two - G_{5_2} and G_{5_4} , can be used to construct parallelisms in general but they cannot be regular. So regular parallelisms with automorphisms of order 5 in $PG(3,5)$ do not exist.

4. References

- [1] Baker, R., Partitioning the planes of $AG_{2m}(2)$ into 2-designs, *Discrete Math* 15, 1976, 205 – 211.
- [2] Betten A., The packings of $PG(3,3)$, *Des. Codes Cryptogr.* 79 (3) 2016, 583 – 595.
- [3] Beutelspacher, A., On parallelisms in finite projective spaces, *Geometriae Dedicata* 3 (1), 1974, 35 – 45.
- [4] Denniston, R. H. F., Some packings of projective spaces, *Atti Accad. Naz. Lincei Rend. Cl. Sci. Fis. Mat. Natur.* 52 (8) 1972, 36 – 40.
- [5] Denniston, R. H. F., Cyclic packings of the projective space of order 8, *Atti Accad. Naz. Lincei Rend. Cl. Sci. Fis. Mat. Natur.* 54 (8) 1973, 373 – 377.
- [6] Eisfeld J., L. Storme, (Partial) t-spreads and minimal t-covers in finite projective spaces. – In: *Lecture notes from the Socrates Intensive Course on Finite Geometry and its Applications*, April 2000, Ghent, Belgium.
- [7] GAP - Groups, Algorithms, Programming - a System for Computational Discrete Algebra (<http://www.gap-system.org/>).
- [8] Johnson, N., *Combinatorics of Spreads and Parallelisms*. Iowa City, CRC Press, 2010.
- [9] Lunardon G., On regular parallelisms in $PG(3,q)$. – *Discrete Mathematics* 51, 1984, 229 – 335.
- [10] Penttila, T. and B. Williams, Regular packings of $PG(3,q)$. – *European J. Combin.* 19 (6) 1998, 713 – 720.
- [11] Prince, A. R., The cyclic parallelisms of $PG(3,5)$. – *European J. Combin.* 19 (5) 1998, 613 – 616.
- [12] Prince A., Covering sets of spreads in $PG(3,q)$, *Discrete Math.* 238, 2001 , 131 – 136.
- [13] Sarmiento, J., Resolutions of $PG(5,2)$ with point-cyclic automorphism group. – *J. Comb. Des.* 8(1) 2000, 2–14.
- [14] Stinson, D., S. Vanstone, Orthogonal packings in $PG(5,2)$. – *Aequationes Math.* 31(1) 1986 , 159–168.
- [15] Storme, L., *Finite Geometry*. – In: *The CRC Handbook of Combinatorial Designs*, CRC Press, second ed., 2006, 702 – 729.
- [16] Topalova, S. and S. Zhelezova, On transitive parallelisms of $PG(3,4)$. – *Appl. Algebra Engrg. Comm. Comput.* 24 (3-4) 2013, 159-164.
- [17] Walker M., Spreads covered by derivable partial spreads. – *Journal of Combinatorial Theory A*, 38 (2), 1985, 113 – 130.

[18] White, C. T., Two cyclic arrangement problems in finite projective geometry: Parallelisms and two intersection set. – PhD thesis, California Institute of Technology, 2002.

[19] Zaicev, G., Zinoviev, V., Semakov, N., Interrelation of Preparata and Hamming codes and extension of Hamming codes to new double-errorcorrecting codes, Proc. of Second Intern. Symp. on Information Theory, (Armenia, USSR, 1971), Budapest, Akademiai Kiado, 1973, 257 – 263.

[20] Zhelezova, S., On regular partial parallelisms of $PG(3,7)$ with automorphisms of order 5. Proc. of scientific conference "25 years Faculty of Mathematics and Informatics – University of Veliko Turnovo", Bulgaria, 2015, to appear.

¹ This research is partially supported by the Bulgarian National Science Fund under Contract No I01/0003

MOLECULAR MODELING AND CREATING 3D MODELS OF CHEMICAL COMPOUNDS IN BLENDER SOFTWARE USING THE RESOURCES OF CHEMSPIDER AND OPEN BABEL

Phd Tihomir Dovramadjiev
Mechanical Engineering Faculty, Industrial Design Department - Technical University of Varna, Bulgaria.
tihomir.dovramadjiev@gmail.com

Abstract: Creating 3D models of molecules and chemical compounds is a necessity in scientific work, which examines different states, structures, processes and interaction of molecules. This is done through the use of comprehensive 3D graphics programs as well as specialized applications containing and maintaining a database of ready-made models. The ability to work with good 3D graphics platform such as Blender combined with available resources of ChemSpider and Open Babel, builds a powerful system allowing the creation of high-quality and realistic virtual models of molecules and chemical compounds.

Keywords: Chemical, molecules, compounds, ChemSpider, Open Babel, Blender

1. Problem discussion

The use of modern technological tools for designing molecules and compounds is an advantage that ensures reliability and speed in the workflow. Very good compatibility to the final modeling in Blender's software [1 - 10] have the utilities ChemSpider [11 - 13] providing molecular resources and Open Babel, as a tool for converting the required file formats [14 - 16]. This study aims to explore possibilities for providing the necessary virtual 3D molecules and chemical compounds used in modern practice and science.

2. Objective and research methodologies

For the purposes of the study a 3D virtual model of Hydroxyapatite (chemical formula $\text{HCa}_5\text{O}_{13}\text{P}_3$) will be provided. This important model is used for creation of computer simulations and animations in Blender environment with support of ChemSpider and Open Babel.

ChemSpider is a freely available database based on chemical structures, that provides information on over 26 million de-duplicated compounds derived from over 400 sources. These sources include a wide variety of government databases, chemical supplier catalogs, academic and commercial websites. Each of the listed sources has a brief popup description, with the full record providing a web link to the source. ChemSpider augments the default information from these sources with additional of property data (official website: <http://www.chemspider.com>). Possibilities of the ChemSpider free chemical database are shown on Fig. 1.



Fig. 1. ChemSpider - the free chemical database. ChemSpider search engine results: Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID

In a real environment $\text{HCa}_5\text{O}_{13}\text{P}_3$ occupies an important place in medicine and implantology in particular, where is applied as a coating and has bioactive function [17 - 19]. Fig. 2 shows 2D view of $\text{HCa}_5\text{O}_{13}\text{P}_3$ and its parameters. Fig. 3 shows 3D image (JSmol) of $\text{HCa}_5\text{O}_{13}\text{P}_3$.

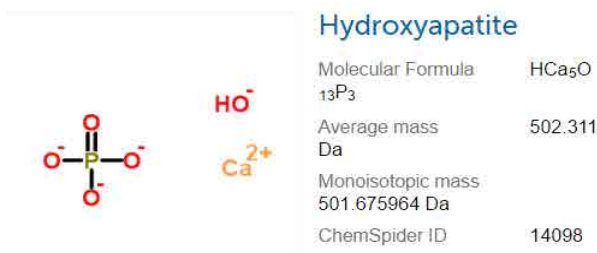


Fig. 2. 2D view of Hydroxyapatite. Molecular Formula $\text{HCa}_5\text{O}_{13}\text{P}_3$. Average mass 502.311 Da Monoisotopic mass 501.675964 Da ChemSpider ID 14098

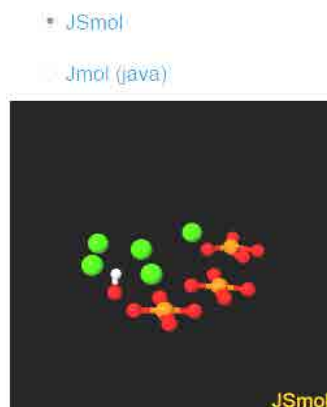


Fig. 3. 3D (JSmol) View of Hydroxyapatite ($\text{HCa}_5\text{O}_{13}\text{P}_3$). (<http://www.chemspider.com/Chemical-Structure.14098.html?rid=376769cf-b675-44b6-b4ed-c475ae68ccce>).

The file from the basis of ChemSpider is downloaded in *.mol format with number 14 098 (as listed in the database). To prepare $\text{HCa}_5\text{O}_{13}\text{P}_3$ model for work first it must be synchronized with the Open Babel (fig. 4) (source Open Babel: An open chemical toolbox).

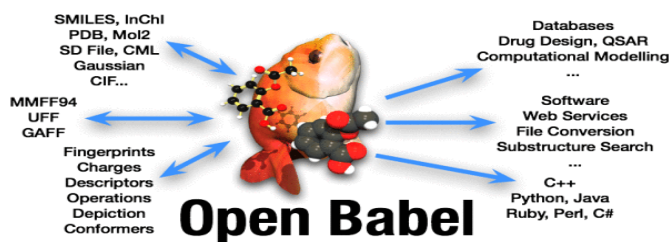


Fig. 4. Open Babel - open source chemical toolbox [14]

Open Babel is a chemical toolbox designed platform which can: search, convert, analyze, or store data from molecular modeling, chemistry, solid-state materials, biochemistry, or related areas. Open Babel is a project to facilitate the interconversion of chemical data from one format to another – including file formats of various types. This is important for the following reasons: multiple programs are often required in realistic workflows; many programs have individual data formats, and/or support only a small subset of other file types; chemical representations often vary considerably (some programs are 2D; some are 3D; some use fractional k-space coordinates; some programs use bonds and atoms of discrete types.; others use only atoms and electrons; some programs use symmetric representations - others do not; some programs specify all atoms - others use "residues" or omit hydrogen atoms). Open Babel Documentation Release 2.3.1. Providing (download) a fully functional open source program Open Babel can be done on the official website <http://openbabel.org/>, following the footsteps. Synchronization of 3D model $\text{HCa}_5\text{O}_{13}\text{P}_3$ obtained from ChemSpider in Open Babel is provided as it is defined in the field "Input format", using format: "mol-- MDL MOL format". The working file is opening with the following data for the model shown in Fig. 4. Processing of $\text{HCa}_5\text{O}_{13}\text{P}_3$ virtual model in PDB is possible by building a 3D coordinate system and determine the location of molecules. In the "Output format", is determined using format: "pdb - Protein Data Bank format". In panel settings are enabled: "Add hydrogens" and "Generate 3D coordinates". Following the conversion data a result is obtained with values shown in Fig. 5.

21.12 0 0000 0 0 0 0 0599 V2000	COMPND UNNAMED
6.1418 -2.2585 0.0000 Ca 0 2 0 0 0 0 0 0 0 0	AUTHOR GENERATED BY OPEN BABEL 2.3.2
6.1418 -2.2585 0.0000 Ca 0 2 0 0 0 0 0 0 0 0	HETATM 1 CA LIG 1 1.056 -0.062 -0.055 1.00 0.00 Ca2+
6.1418 -2.2585 0.0000 Ca 0 2 0 0 0 0 0 0 0 0	HETATM 2 CA LIG 2 1.056 -0.062 -0.055 1.00 0.00 Ca2+
6.1418 -2.2585 0.0000 Ca 0 2 0 0 0 0 0 0 0 0	HETATM 3 CA LIG 3 1.056 -0.062 -0.055 1.00 0.00 Ca2+
6.1418 -2.2585 0.0000 Ca 0 2 0 0 0 0 0 0 0 0	HETATM 4 CA LIG 4 1.056 -0.062 -0.055 1.00 0.00 Ca2+
1.2861 -1.9950 0.0000 P 0 0 0 0 0 0 0 0 0 0	HETATM 5 CA LIG 5 1.056 -0.062 -0.055 1.00 0.00 Ca2+
1.2861 -1.9950 0.0000 P 0 0 0 0 0 0 0 0 0 0	HETATM 6 P LIG 6 1.056 -0.062 -0.055 1.00 0.00 P
1.2861 -1.9950 0.0000 P 0 0 0 0 0 0 0 0 0 0	HETATM 7 P LIG 7 1.056 -0.062 -0.055 1.00 0.00 P
1.2861 -1.9950 0.0000 P 0 0 0 0 0 0 0 0 0 0	HETATM 8 P LIG 8 1.056 -0.062 -0.055 1.00 0.00 P
1.2861 -1.9950 0.0000 O 5 0 0 0 0 0 0 0 0 0	HETATM 9 O LIG 6 1.056 -0.062 -0.055 1.00 0.00 O1-
1.2861 -1.9950 0.0000 O 5 0 0 0 0 0 0 0 0 0	HETATM 10 O LIG 6 1.056 -0.062 -0.055 1.00 0.00 O1-
1.2861 -1.9950 0.0000 O 5 0 0 0 0 0 0 0 0 0	HETATM 11 O LIG 6 -0.574 -0.062 -0.055 1.00 0.00 O1-
1.2861 -1.9950 0.0000 O 5 0 0 0 0 0 0 0 0 0	HETATM 12 O LIG 7 1.056 -0.062 -0.055 1.00 0.00 O1-
1.2861 -1.9950 0.0000 O 5 0 0 0 0 0 0 0 0 0	HETATM 13 O LIG 7 1.056 -1.209 1.241 1.00 0.00 O1-
1.2861 -1.9950 0.0000 O 5 0 0 0 0 0 0 0 0 0	HETATM 14 O LIG 7 -0.574 -0.062 -0.055 1.00 0.00 O1-
1.2861 -1.9950 0.0000 O 5 0 0 0 0 0 0 0 0 0	HETATM 15 O LIG 8 1.056 -0.062 -0.055 1.00 0.00 O1-
1.2861 -1.9950 0.0000 O 5 0 0 0 0 0 0 0 0 0	HETATM 16 O LIG 8 1.056 -1.209 1.241 1.00 0.00 O1-
1.2861 -1.9950 0.0000 O 5 0 0 0 0 0 0 0 0 0	HETATM 17 O LIG 8 -0.574 -0.062 -0.055 1.00 0.00 O1-
1.2861 -0.6650 0.0000 O 0 0 0 0 0 0 0 0 0 0	HETATM 18 O LIG 6 2.601 -0.062 -0.055 1.00 0.00 O
1.2861 -0.6650 0.0000 O 0 0 0 0 0 0 0 0 0 0	HETATM 19 O LIG 7 2.601 -0.062 -0.055 1.00 0.00 O
1.2861 -0.6650 0.0000 O 0 0 0 0 0 0 0 0 0 0	HETATM 20 O LIG 8 2.601 -0.062 -0.055 1.00 0.00 O
6.2736 0.0000 0.0000 O 5 0 0 0 0 0 0 0 0 0	HETATM 21 O HOH 9 1.056 -0.062 -0.055 1.00 0.00 O1-
6.9 1 0	HETATM 22 H HOH 0 2.035 -0.062 -0.055 1.00 0.00 H
6.10 1 0	CONNECT 6 9 10 11 18
6.11 1 0	CONNECT 6
6.18 2 0	CONNECT 7 12 13 14 19
7.12 1 0	CONNECT 7
7.13 1 0	CONNECT 8 15 16 17 20
7.14 1 0	CONNECT 8
7.19 2 0	CONNECT 9
8.15 1 0	CONNECT 9 6
8.16 1 0	CONNECT 10 6

Fig. 5. Open Bible data conversation (a) Input format: mol-- MDL MOL format of $\text{HCa}_5\text{O}_{13}\text{P}_3$ (b) . Output format: pdb -- Protein Data Bank format of $\text{HCa}_5\text{O}_{13}\text{P}_3$.

The resulting data is saved in a file with the extension *.PDB. (HA.PDB). The file is imported into Blender software, through activation of Atomic Blender - PDB Addon (File → User Preferences → Import-Export Atomic Blender - PDB). The file containing the data for $\text{HCa}_5\text{O}_{13}\text{P}_3$ is used for simulations, animations and visualizations for assignment. Fig.6(a) shows the configuration of the defined $\text{HCa}_5\text{O}_{13}\text{P}_3$ and Fig.6(b) shows visualization of 3D models in Blender's environment.

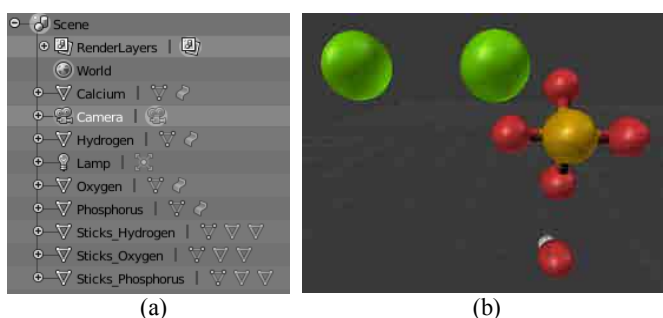


Fig. 6. 3D model of $\text{HCa}_5\text{O}_{13}\text{P}_3$ in Blender's environment (a) configuration (b) visualization

Using the same methodology other molecules and compounds can be used, to be added to the existing ones, to be modified and examined.

3. Conclusion

Finding and using available open source reservoirs which have data for the needs of modern science, and especially biology, medicine, biomedicine, chemistry and others is particularly relevant at the moment. This is possible due to the rapidly increasing volume of information, delivery to accessible repositories of information and easy access. A very good example is ChemSpider, where incoming information data is scientifically confirmed. On the other side the data is easily converted to Open Babel and becomes fit for further research in Blender software, which allows to carry out many successful actions and developments on assignment.

References

- [1]. Tihomir Dovramadjiev. Modern accessible application of the system blender in 3d design practice. International scientific on-line journal "SCIENCE & TECHNOLOGIES" Publisher "Union of Scientists - Stara Zagora". ISSN 1314-4111 140. Bulgaria, 2015. 10 - 13p.
- [2]. Felician Alecu, Blender Institute – the Institute for Open 3D Projects, Open Source Science Journal Vol. 2, No. 1, Economic Informatics Department, ASE Bucharest, Romania, 2010, 36 – 45p.
- [3]. Ami Chopine, 3D Art Essentials The Fundamentals of 3D Modeling, Texturing, and Animation, Elsevier, ISBN: 978-0-240-81471-1, USA, 2011, 249 – 252p.
- [4]. John M. Blain. Computer Modeling and Animation. The Complete Guide to Blender Graphics. Taylor & Francis Group, LLC. ISBN:13- 978-1-4665-1704-2. UK, 2012.
- [5]. A.A.Прахов, Blender: 3D-моделирование и анимация. СПб.: БХ В, ISBN 978-5-9775-0393-8, Русия, 2009, 272 с: ил.
- [6]. Ami Chopine, 3D Art Essentials The Fundamentals of 3D Modeling, Texturing, and Animation, Elsevier, ISBN: 978-0-240-81471-1, USA, 2011, 249 – 252.
- [7]. Felician Alecu, Blender Institute – the Institute for Open 3D Projects, Open Source Science Journal Vol. 2, No. 1, Economic Informatics Department, ASE Bucharest, Romania, 2010, 36 – 45.
- [8]. James Chronister, Blender 3D Basics 3rd Edition, Creative commons attribution NonCommercial-share alike 3.0 Unported License, 2009, 146 p.
- [9]. Lance Flavell, Beginning Blender - Open Source 3D Modeling, Animation, and Game Design, Apress, ISBN-13 (pbk): 978-1-4302-3126-4, USA, 2010.
- [10]. Roger D. Wickes, Foundation Blender Compositing, ISBN-13 (pbk): 978-1-4302-1976-7, USA, 2009.
- [11]. Pence, H. E. & Williams, A. (2010). ChemSpider: An Online Chemical Information Resource, Journal of Chemical Education 87 : 1123-1124.
- [12]. Crystallography Open Database (COD). Vilnius University Press. 2014. 12-13p.
- [13]. M. Rabie and C. M. Franck. Predicting the electric strength of proposed sf6 replacement gases by means of density functional theory. 18th Int. Simp. of high voltage engineering. South Korea, 2013. 1381 - 1386p.
- [14]. Noel M. O'Boyle. Open Babel. Access and interconvert chemical information. Open Babel development team and NextMove Software. Cambridge, UK, 2013. 39p.
- [15]. Enade Perdana Istyastono. Construction and optimization of structure-based virtual screening protocols to identify cyclooxygenase-1 inhibitors using Open Babel, spores and plants. Indo. J. Chem., Indonesia 2012, 12 (2), 141 - 145p.
- [16]. Geoffrey R Hutchison Chris Morley Craig James Chris Swain Hans De Winter Tim Vandermeersch Noel M O'Boyle (Ed.). Open Babel Documentation. Release 2.3.1. 2012. 145p.
- [17]. Abdulaziz Binahmed, Andrew Stoykewych, Ali Hussain, Brock Love, Vijay Pruthi. Long-Term Follow-up of Hydroxyapatite-Coated Dental Implants—A Clinical Trial. The International Journal of Oral & Maxillofacial Implants. Quintessence Publishing Co. 2007, 963 - 968 p.
- [18]. A. Jemat, M. J. Ghazali, M. Razali and Y. Otsuka. Surface Modifications and Their Effects on Titanium Dental Implants. Hindawi Publishing. Egypt, 2015. 11p.
- [19]. A. Simunek, D Kopecka, M Cierny, I Krulichova. A Six-Year Study of Hydroxyapatite-Coated Root-Form Dental Implants. West Indian Med J 2005; 54 (6): 393 - 397p.

MOLECULAR SIMILARITY IN THE FRAMEWORK OF A BIOISOSTERISM STUDY

ИЗСЛЕДВАНЕ НА МОЛЕКУЛЯРНА СЪВМЕСТИМОСТ В СРЕДА НА БИОИЗОСТЕРИЗЪМ

Desislava Ivanova

ИСТ – BAS

divanovaacomin@gmail.com

Abstract: *Bioisosterism is a strategy of Medicinal Chemistry for the rational design of new drugs (bioisosterism is also known as quantum similarity). The success of this strategy in developing new substances which are therapeutically attractive has observed a significant growth in distinct therapeutic classes, being amply used by the pharmaceutical industry to discover new analogs of therapeutic innovations commercially attractive, and also as a tool useful in the molecular modification. In this work, the concept of quantum similarity in the signed particle formulation of quantum mechanics is introduced. This concept was suggested very recently and was studied for the particular case $n=1$. Therefore, we extend the mathematical expression of similarity to the case $n>1$, with particular attention to the differences brought in this new context.*

Keywords: QUANTUM SIMILARITY, MOLECULAR DESCRIPTOR, BIOISOSTERISM.

1. Introduction

The notion of molecular quantum similarity was proposed in 1980 and, since then, a growing interest has been shown towards this concept [1]. As a matter of fact, nowadays it is utilized for practical purposes in many different fields such as organic, quantum and physical chemistry. It is interesting to note that different definitions of a quantum similarity can be provided depending on the context. For example, organic chemists may define two similar molecules when they have similar reactivity in certain reactions, while quantum chemists may focus on the molecular features, etc. Therefore, it is not surprising that it is difficult, if not impossible, to provide a universal definition of quantum similarity. In spite of that, it is important to have a practical definition even though it may be related to a particular context. For instance, in a pharmaceutical context molecular quantum similarity may provide a systematic way to investigate the relation between the structure of a molecule and its chemical reactivity, thus drastically easing the process of drug design and minimizing the occurrence of side effects.

While the concept of quantum similarity is becoming widespread in many communities and different definitions are being provided, to the best of our knowledge it seems that all directions taken so far are based on the Schrödinger (or standard) formulation of quantum mechanics [2]. However, different formulations exist which may offer a different perspective on the concept of quantum similarity [3–7]. In practice, in order to concretely (mathematically) define the concept of molecular quantum similarity, one has to define a molecular descriptor first. While an infinite set of options is available, for many practical and theoretical reasons, the electron density has become the most common choice [1].

Recently, a new definition of quantum similarity has been proposed based on the concept of quasi-distribution functions [8]. This novel approach exploits the Wigner formulation of quantum mechanics which belongs to the class of phase-space formalisms and has been implemented in the framework of the Wigner Monte Carlo method [8]. On the other hand, a new formulation of quantum mechanics has recently been suggested which is based on the intuitive concept of (signed) classical particles [10]. These particles are contemporaneously provided with a position and a momentum, and therefore this formalism belongs to the class of phase-space formulations of quantum mechanics. In particular, it is able to reconstruct the corresponding Wigner quasi-distribution function of a given quantum system which, in turn, represents the molecular indicator chosen in [8]. Again, one should note that the common molecular indicator utilized in quantum chemistry is represented in the vast majority of studies by the probability density in the real

space (also referred to as electronic structure). While our definition of quantum similarity is a drastic departure from the common definition, the reader should also note that it actually corresponds to its generalization.

2. Bioisosterism

Bioisosterism is a strategy of Medicinal Chemistry for the rational design of new drugs (see reference [1] below, bioisosterism is also known as quantum similarity). The success of this strategy in developing new substances which are therapeutically attractive has observed a significant growth in distinct therapeutic classes, being amply used by the pharmaceutical industry to discover new analogs of therapeutic innovations commercially attractive, and also as a tool useful in the molecular modification. A way to achieve reliable bioisosteric analysis is by means of quantum simulation of given molecules. As a matter of fact, without simulation capabilities, this analysis would be limited to experimental observations which cannot always be provided, not to mention the high cost of such experiments. Furthermore, quantum simulations allow researchers to access to an amount of details which is practically impossible nowadays. Indeed, energy levels, electronic structure, molecular orbitals, exchange-correlation energies (just to mention a few of them) cannot be easily measured with the actual laboratory technology.

While quantum simulations for the study of bioisosterism is already available the visualization of the results obtained from these simulations is still a tricky and complex task. Indeed, it is clear that the use of a three-dimensional screen would strongly improve the understanding of bioisosteric molecules. What remains to be clarified is the way visualizations should be done to obtain an intuitive and efficient analysis. Furthermore, one of the main outcome of this investigation would be the development of a know-how that could be utilized by physicists and chemists for this particular kind of chemical/medical investigation. Finally, at least one publication about the developed technique would be published in a peer reviewed international scientific journal. An important aspect of this publication may be represented by the potential of attracting pharmaceutical and medical companies. Several simulation will be ran and a couple of several numerical experiments will be performed in order to validate the new definition. A set of molecules and crystal structures which could be used to benchmark this new framework. One of these could be the Graphene, Silicene and Titanium Dioxide which have an incredible amount of possible applications (Graphene is raising a lot of interest as one of the European H2020 Flagship Projects). The task is to create a three-dimensional visualization of meaningful molecular

orbitals which vibrate in a way which is not visible on a normal screen. This opens the door towards real-time three-dimensional visualization and manipulation of quantum objects.

A way to achieve reliable bioisosteric analysis is by means of quantum simulation of given molecules. As a matter of fact, without simulation capabilities, this analysis would be limited to experimental observations which cannot always be provided, not to mention the high cost of such experiments. Furthermore, quantum simulations allow researchers to access to an amount of details which is practically impossible nowadays. Indeed, energy levels, electronic structure, molecular orbitals, exchange-correlation energies (just to mention a few of them) cannot be easily measured with the actual laboratory technology. While quantum simulations for the study of bioisosterism is already available the visualization of the results obtained from these simulations is still a tricky and complex task. Indeed, it is clear that the use of a three-dimensional screen would strongly improve the understanding of bioisosteric molecules. What remains to be clarified is the way visualizations should be done to obtain an intuitive and efficient analysis. Furthermore, one of the main outcome of this investigation would be the development of a know-how that could be utilized by physicists and chemists for this particular kind of chemical/medical investigation. Finally, at least one publication about the developed technique would be published in a peer reviewed international scientific journal. An important aspect of this publication may be represented by the potential of attracting pharmaceutical and medical companies.

3. Molecular descriptor

In more details, in order to mathematically define the concept of molecular quantum similarity in a particular context, one must first select a significant molecular descriptor. In practical applications, this descriptor will depend on the particular simulated system and on the specific task one wants to achieve. Thus, a universal choice good for any situation is simply not possible.

In practice, one may arrange the most common descriptors in use nowadays in several main classes [10]:

- Feature counts. This is the simplest class of descriptors which consists of counting a certain feature in a molecule. An example is represented by the number of certain atomic species in a molecule.
- Physicochemical parameters. In this class, one finds the descriptors defined in terms of specific physical and/or chemical features. A good example is the partition coefficient (logP).
- Fragment descriptors. These descriptors are based on molecular two-dimensional connection tables and three-dimensional descriptions of the structure for substructure searches.
- Topological indices. This represents a wide range of atom based descriptors expressed in terms of indices. Examples are represented by the Wiener index (sometimes referred to as Wiener number).
- Field-based descriptors. Descriptors in this class are based on fields such as the electron density, the electrostatic potential, etc. This represents, at the present time, the frontline in the field of molecular quantum similarity. These descriptors can be subdivided into two sub-categories: measurable and non-measurable.
- Others. Further classes can be given [11].

Although the list of descriptors seems to be enormous, to the best of our knowledge, it seems that they all have one thing in common: they are all based on the Schrödinger formulation of quantum mechanics. No attempt to define a molecular descriptor and, thus, the notion of a molecular quantum similarity in the context of the Wigner formalism seems to have been done. Moreover, the electron density $\rho(x)$ appears, so far, to play a fundamental role in the definition of molecular quantum similarity (note that the density is usually time-independent in this context).

The focus is aimed at on defining a molecular descriptor based on the Wigner quasi-distribution function $f_W = f_W(x; p; t)$, and we investigate the possible advantages in doing so (note that the function f_W is time-dependent). In this respect, we define a new field-based molecular descriptor.

In a previous research of the author was found an intuitive definition of quantum similarity which is expressed in terms of distribution functions (in the Wigner formalism) instead of a simple probability density function (as it is done usually in other formulations of quantum mechanics). In particular, a great deal of attention has been put in the visualization of the multi-dimensional distribution functions to understand what quantities should be properly exploited. The new definition defines the similarity of two quantum systems by means of the similarity they achieve in the multi-dimensional phase-space. In practice, our new definition of quantum similarity based on the utilization of quasi-distribution functions reads:

$$d_{AB}^n(t) = \int dx \int dp \left| \left(f_W^A(x; p; t) \right)^n - \left(f_W^B(x; p; t) \right)^n \right|^{\frac{1}{n}}$$

with n an integer (taken equal to 1 in [8]). It is trivial to see that, by simulating quantum systems by means of the signed particle formulation, one can reconstruct the quasi-distribution function of two given systems and, therefore, compute their similarity.

As a matter of fact, after running several simulations, it became quickly clear that a definition in the phase-space brings several non-negligible advantages. In fact, the existence of systems which would be considered similar when the old definition is applied, but very different when the new definition is applied (because they are not similar energetically speaking) was discovered. By means of visualization tools, in particular VisIt (LLNL) and paraview (Kitware), it was possible to explain why the new definition is actually superior.

Finally, several numerical experiments have been performed in order to further validate the new definition, focusing on simple controllable chemical systems such as a free electron in vacuum and the H2 molecule, and, in order to keep the concepts simple and clear, the validation is performed between the initial conditions and the actual conditions of a quantum system. The results clearly show that the new definition is, at least in several cases, superior.

In this project, we want to focus on the above formula and modify the integer $n=1$ to $n=2, 3, 4$. We observe that different values of this integer brings different ways of measuring the quantum similarity between two (or more) quantum systems. Such investigation will not only help us to understand what is the best possible mathematical expression of quantum similarity in the context of phase-space formulations of quantum mechanics, it will also offer a practical tool exploitable by chemistry base companies such as, for instance, pharmaceutical companies, electronics, materials, etc.

In practice, we mathematically define the new molecular quantum similarity in the following way. Given two molecules A and B described, respectively, by the quasi-distribution functions f_W^A and f_W^B , their quantum similarity is defined as:

$$d_{AB}(t) = \int dx \int dp \left| f_W^A(x; p; t) - f_W^B(x; p; t) \right|$$

where the integration is performed over the phase-space simulation domain. Obviously, this is not the only possible choice and one may consider the definition above as a special case of

$$d_{AB}^n(t) = \int dx \int dp \left| \left(f_W^A(x; p; t) \right)^n - \left(f_W^B(x; p; t) \right)^n \right|^{\frac{1}{n}}$$

with $n = 1$. It is clear from this definition that $d_{AB} \geq 0$ and two molecules are said to be similar only when their distance d_{AB} is close or equal to zero. Conversely, the bigger the number $d_{AB}(t)$ the less similar the molecules are.

The quantum system taken into account for our numerical experiments consists of an hydrogen atom in the Bohr-Oppenheimer approximation. This system is considered going from the ground state and vice versa and the quantum similarity between this two states is computed in function of time. Fig. 1 shows what the orbitals of an electron in such system look like (these results are obtained by means of the signed particle formulation [2]). In particular, the left-hand side shows the electron in the 1s state while the right-hand side shows the same electron in the 2s state.

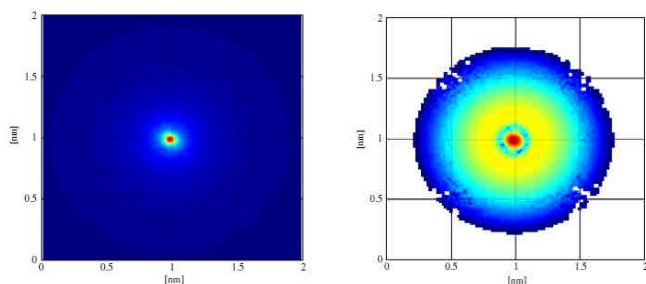


Fig. 1 Electronic orbitals in a hydrogen atom corresponding to 1s and 2s

4. Results

A wide range of outcomes is expected. As a preliminary application of our suggested approach, we show in Fig.2 the similarity in time coming from a system of Gaussian wave-packets interacting with an external potential [1].

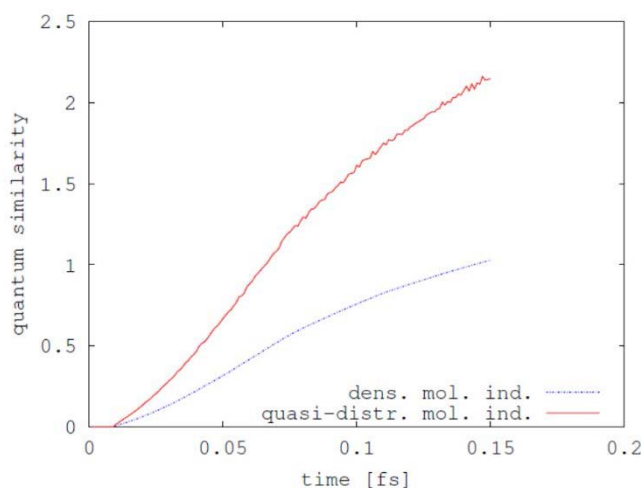


Fig.2 Comparison of quantum similarities with two different molecular descriptors for a H2 molecule. The dashed (blue) curve corresponds to the density probability as the molecular descriptor, while the continuous (red) curve corresponds to the quasi-distribution function as the descriptor [1].

Acknowledgments

The work is supported by the "Research program for young scientists at the Bulgarian Academy of Science 2016 funded by the Bulgarian Ministry of Education and Science - Bulgaria National Science Fund under grant DFNP - 101/04.05.2016

References

- [1] R. Carbo, J. Arnau, L. Leyda, How similar is a molecule to another? An electron density measure of similarity between two molecular structures, *Int. J. Quantum Chem.* 17 (1980) 1185.
- [2] E. Schrödinger, Quantisierung als Eigenwertproblem, *Ann. Phys.* 385 (1926) 437–490.
- [3] E. Wigner, On the quantum correction for thermodynamic equilibrium, *Phys. Rev.* 40 (1932) 749.
- [4] R.P. Feynman, Space–time approach to non-relativistic quantum mechanics, *Rev. Modern Phys.* 20 (1948) 367.
- [5] L.V. Keldysh, *Zh. Eksp. Teor. Fiz., Sov. Phys. JETP* 20 (1965).
- [6] K. Husimi, Some formal properties of the density matrix, *Nippon Sugaku-Buturigakkwai Kizi Dai* 3 Ki 22 (4) (1940) 264–314.
- [7] D. Bohm, A suggested interpretation of the quantum theory in terms of hidden variables. I, *Phys. Rev.* 85 (1952) 166.
- [8] J.M. Sellier, D.Y. Ivanova, I. Dimov, *Molecular Descriptors and Quasi-distribution Functions, Computers and Mathematics with Applications, Elsevier, Volume 70, Issue 11, Pages 2726–2731, (2015).*
- [9] Sellier, J.M., Ivanova, D. Y., Dimov, I. (2016). "A study on quantum similarity in the phase space". *Physica A: Statistical Mechanics and its Applications* 460: 116 - 120. doi:10.1016/j.physa.2016.05.003
- [10] J.M. Sellier, A Signed Particle Formulation of Non-relativistic Quantum Mechanics, *Journal of Computational Physics, Elsevier, Volume 297, Pages 254–265, (2015).*
- [11] G.M. Downs, in: P. Bultinck, H. De Winter, W. Langenaeker, J.P. Tollenaere (Eds.), *Computational Medicinal Chemistry for Drug Discovery, Dekker, Inc., New York, 2003, pp. 364–386. Molecular Descriptors.*

SOFTWARE DESIGN

M.Sc. Ivanova Milka

Faculty of Mechanical Engineering – Technical University of Sofia, Bulgaria

milkachr@tu-sofia.bg

Abstract: *As a process, software design is the software engineering life cycle activity in which software requirements are analyzed in order to produce a description of the software's internal structure that will serve as the basis for its construction. A software design (as the result) describes the software architecture-that is, how software is decomposed and organized into components-and the interfaces between those components*

In the report they have explained breakdown of topics of process of software design

Keywords: SOFTWARE STRUCTURE& DESIGN&ARCHITECTURE, INTERFACE DESIGN, SOFTWARE QUALITY, SOFTWARE DESIGN METHODS&STRATEGIES, SOFTWARE DESIGN TOOLS, SOFTWARE STANDARDS

Design is defined as[7], both "the process of defining the architecture, components, interfaces, and other characteristics of a system or component" and "the result of [that] process". Software design plays an important role in developing software: it allows software engineers to produce various models that form a kind of blueprint of the solution to be implemented

As a process, software design is the software engineering life cycle activity in which software requirements are analyzed in order to produce a description of the software's internal structure that will serve as the basis for its construction. A software design (as the result) describes the software architecture-that is, how software is decomposed and organized into components-and the interfaces between those components.

In a standard IEEE Std 12207 Software Life Cycle Processes software life cycle processes, such as [1], software design consists of two activities that fit between software requirements analysis and software construction:

- ◆ Software architectural design (top-level design): describing software's top-level structure and organization and identifying the various components;
- ◆ Software detailed design: describing each component sufficiently to allow for its construction.

The current Software Design Knowledge Area (KA) description does not discuss every topic whose name contains the word "design." The KA discussed in this chapter deals mainly with D-design (decomposition design, whose goal is to map software into component pieces); FP-design (family pattern design, whose goal is to establish exploitable commonalities in a family of software). By contrast, the Software Design KA does not address I-design (invention design, which is performed during the software requirements process with the goal of conceptualizing and specifying software to satisfy discovered needs and requirements). The Software Design KA description is related specifically to Software Requirements, Software Construction, Software Engineering Management, Software Engineering Models and Methods, Software Quality, and Computing Foundations KAs.

1. Software Design Fundamentals The concepts, notions, and terminology introduced here form an underlying basis for understanding the role and scope of software design.

1.1 General Design Concepts

Software is not the only field where design is involved. In the general sense, we can view design as a form of problem solving. The concept of a wicked problem-a problem with no definitive solution-is interesting in terms of understanding the limits of design. A number of other notions and concepts in its general sense are goals, constraints, alternatives, representations, and solutions.

1.2 Context of Software Design

The role of software design it is important to understand the context in which it fits: the software engineering life cycle. It is important to understand the major characteristics of software requirements

analysis vs. software design vs. software construction vs. software testing.

1.3 Software Design Process

Software design is generally considered a two-step process: Architectural design which describes how software is decomposed and organized into components and Detailed design which describes the specific behavior of these components.

1.4 Software Design Principles

Software design principles are key notions considered fundamental to many different software design approaches and concepts. Software design principles include abstraction, coupling, and cohesion; decomposition and modularization; encapsulation / information hiding; separation of interface and implementation; sufficiency, completeness, and primitiveness; and separation of concerns.

- ◆ Abstraction is "a view of an object that focuses on the information relevant to a particular purpose and ignores the remainder of the information". In the context of software design, they are two key abstraction mechanisms: parameterization and specification. Abstraction by specification leads to three major kinds of abstraction: procedural abstraction, data abstraction, and control (iteration) abstraction.
- ◆ Coupling and cohesion are defined as "a measure of the interdependence among modules in a computer program," whereas cohesion is defined as "a measure of the strength of association of the elements within a module".
- ◆ Decomposition and modularization mean that large software are divided into a number of smaller independent ones, usually with the goal of placing different functionalities or responsibilities in different components.
- ◆ Encapsulation/information hiding means grouping and packaging the elements and internal details of an abstraction and making those details inaccessible.
- ◆ Separation of interface and implementation involve defining a component by specifying a public interface (known to the clients) that is separate from the details of how the component is realized.
- ◆ Sufficiency, completeness and primitiveness mean ensuring that a software component captures all the important characteristics of an abstraction and nothing more
- ◆ Separation of concerns suggests that any complex problem can be more easily handled if it is subdivided into pieces that can each be solved and/or optimized independently. A concern is an "area of interest with respect to a software design" [5]. By separating concerns into smaller-and therefore more manageable-pieces, a problem takes less effort and time to solve.

2. Key Issues in Software Design A number of key issues must be dealt with when designing software. This is how to decompose, organize, and package software components. This is so fundamental that all design approaches must address it in one way or another. In contrast, other issues "deal with some aspect of software's behavior

that is not in the application domain, but which addresses some of the supporting domains" [4]. Such issues, which often cross-cut the system's functionality, have been referred to as *aspects*, which "tend not to be units of software's functional decomposition, but rather to be proper-ties that affect the performance or semantics of the components in systemic ways" [2].

2.1. *Concurrency* looks at how to decompose the software into processes, tasks, and threads and deal with related efficiency, atomicity, synchronization, and scheduling issues.

2.2. *Control and Handling of Events* looks at how to organize data and control flow as well as how to handle reactive and temporal events through various mechanisms such as implicit invocation and call-backs.

2.3. *Data Persistence* looks at how to handle long-lived data.

2.4. *Distribution of Components* looks at how to distribute the software across the hardware, how the components communicate, and how middleware can be used to deal with heterogeneous software.

2.5. *Error and Exception Handling and Fault Tolerance* looks at how to prevent and tolerate faults and deal with exceptional conditions.

2.6. *Interaction and Presentation* looks at how to structure and organize interactions with users as well as the presentation of information. This topic does not specify user interface details, which is the task of user interface design.

2.7. *Security* looks at how to prevent unauthorized disclosure, creation, changing, deleting or denying of information and other resources; and how to tolerate security-related attacks or violations by limiting damage, continuing service, speeding repair and recovery, and failing and recovering securely. Access control is fundamental so much of security; one must also ensure the proper use of cryptology.

3 Software Structure and Architecture In its strict sense, software architecture is "the set of structures needed to reason about the system, which comprise software elements, relations among them, and properties of both" [3]. Architecture attempts to define the internal structure of the resulting software. During the mid-1990s software architecture started to emerge as a broader discipline that involved the study of software structures and architectures in a more generic way. This gave rise to a number of interesting ideas about software design at different levels of abstraction. Some of these concepts can be useful during the architectural design (for example in architectural style) of specific software as well as during the detailed design (for example in lower-level design patterns) of that software. But they can also be useful for designing generic software, leading to the design of families of programs (also known as product lines).

3.1. *Architectural Structures and Viewpoints* are different high-level facets of a software design can and should be described and documented. These are called *views*: "A view represents a partial aspect of a software architecture that shows specific properties of a software system" [3]. These distinct views pertain to distinct issues associated with software design—for example, the logical view (satisfying the functional requirements) vs. the process view (concurrency issues) vs. the physical view (distribution issues) vs. the development view (how the design is broken down into implementation units).

3.2. *Architectural Styles* are "a specialization of element and relation types, together with a set of constraints on how they can be used" [3]. An architectural style can thus be seen as providing the software's high-level organization. Various authors have identified a number of major architectural styles.

- ◆ General structure layers, pipes, filters, blackboard
- ◆ Distributed systems: client-server, three-tiers, broker
- ◆ Interactive systems: Model-View-Controller, Presentation-Abstraction-Control
- ◆ Adaptable systems: micro-kernel, reflection
- ◆ Others: for example, batch, interpreters, process control, rule-based).

3.3. *Design Patterns described*, a pattern is "a common solution to a common problem in a given context" [6]. While architectural styles

can be viewed as patterns describing the high-level organization of software, other design patterns can be used to describe details at a lower, more local level (their microarchitecture).

- ◆ Creational patterns: builder, factory, prototype, singleton
- ◆ Structural patterns: adapter, bridge, composite, decorator, facade, flyweight, proxy
- ◆ Behavioral patterns: command, interpreter, iterator, mediator, memento, observer, state, strategy, template, visitor

3.4. *Architecture Design Decisions* are a creative process. During this process, software architects have to make a number of fundamental decisions that profoundly affect the software and its development process. It is more useful to think of the architectural design process from a decision perspective rather than from an activity perspective.

3.5. *Families of Programs and Frameworks* is one possible approach to allow the reuse of software designs and components to design families of software, also known as software product lines. This can be done by identifying the commonalities among members of such families and by using reusable and customizable components to account for the variability among family members

4. User Interface Design User interface design is an essential part of the software design process. To achieve software's full potential, its user interface should be designed to match the skills, experience, and expectations of its anticipated users.

4.1 *General User Interface Design Principles*

- ◆ Learnability. The software should be easy to learn so that the user can rapidly start getting some work done with the software.
- ◆ User familiarity. The interface should use terms and concepts drawn from the experiences of the people who will make most use of the software.
- ◆ Consistency. The interface should be consistent so that comparable operations are activated in the same way.
- ◆ Minimal surprise. The behavior of software should not surprise users.
- ◆ Recoverability. The interface should provide mechanisms allowing users to recover from errors.
- ◆ User guidance. The interface should give meaningful feedback when errors occur and provide context-related help to users.
- ◆ User diversity. The interface should provide appropriate interaction mechanisms for different types of users.

4.2 *User Interface Design Issues*

User interface design should solve two key issues:

- (1) How should the user interact with the software?
- (2) How should information from the software be presented to the user?

User interface must integrate user interaction and information presentation. User interface design should consider a compromise between the most appropriate styles of interaction and presentation for the software, the background and experience of the Software users, and the available devices.

4.3 *The Design of User Interaction Modalities*

User interaction means issuing commands and associated data to the software. User interaction styles can be classified into the primary styles as follows.

- ◆ Question-answer. The interaction is essentially restricted to a single question-answer exchange between the user and the software. The user issues a question to the software, and the software returns the answer to the question. It is line-oriented.
- ◆ Direct manipulation. Users interact directly with objects on the screen. Direct manipulation often includes a pointing device (such as a mouse, trackball, or finger on touch screens) that guides the manipulated object and action that specifies what should be done with
- ◆ Menu selection. The user selects a command from a menu list of commands.
- ◆ Form fill-in. The user fills in the fields of a form. Sometimes fields include menus, in which case the form has action buttons for the user to initiate action.
- ◆ Command language. The user issues a command and related parameters to direct the software what to do.

- ◆ Natural language. The user issues a command in natural language. That is, the natural language is a front end to a command language and is parsed and translated to software commands.

4.4 The Design of Information Presentation

Software often needs to provide some way of presenting information to users. Such information presentation may be a direct representation of the input information or it may be graphical information. A good design should keep the information presentation separate from the information itself. Software engineers must consider software response time and feedback in the design of information presentation. Software response time is generally measured from the point at which a user executes a certain control action until the software responds with the desired output or response. Before the software returns the desired response, it should give feedback on what the software is doing. Software feedback should not be expressed in abstract and general terms but should restate and rephrase the user's input to indicate what processing is being completed from this input. When large amounts of information have to be presented, abstract visualizations that link data items can be used. According to the style of information presentation, designers should think about how to color the interface. There are several important guidelines, which follow.

- ◆ Limit the number of colors used.
- ◆ Use color change to show the change of software status.
- ◆ Use color coding to support the user's task.
- ◆ Use color coding in a thoughtful and consistent way.

4.5 User Interface Design Process

User interface design is an iterative process; interface prototypes are often used to decide the features, organization, and look of the software user interface. This process includes three core activities:

- ◆ User analysis. In this phase, the designer should analyze the users' tasks, working environment, and other software as well as how users interact with other people.
- ◆ Software prototyping. Developing prototype software and exposing them to users can guide the evolution of the interface.
- ◆ Interface evaluation. Designers can formally evaluate users' actual experiences with the interface.

4.6 Localization and Internationalization

User interface design needs to consider internationalization and localization, which are means of adapting software to the different languages, regional differences, and technical requirements of a target market. Internationalization is the process of designing a software application so that it can be adapted to various languages and regions without engineering changes. Localization is the process of adapting internationalized software for a specific region or language by adding locale-specific components and translating text. Localization and internationalization should notably consider characters, numbers and currency, time and measurement units.

4.7 Metaphors and Conceptual Models

User interface design often needs to set up the mappings between the information display and the user's conceptual model of the information. User interface design can use interface metaphors to set up a mapping between the software and some reference system known to the users in the real world in order to help them to learn and use the interface. For example, the operation "delete file" can be metaphorized as the icon of a trash can in user interfaces. When designing a user interface, software engineers should pay attention to not imply more than one intended metaphor. Metaphors also present potential problems with respect to internationalization, since not all metaphors are meaningful or not in the same way to all cultures.

5. Software Design Quality Analysis and Evaluation This includes a number of quality and evaluation topics that are specifically related to software design.

5.1. Quality Attributes

Various attributes are generally considered important for obtaining a software design of good quality-various "utilities" (maintainability, portability, testability, traceability) and "nesses" (correctness, robustness), including "fitness of purpose." There is an interesting distinction between quality attributes discernible at run-time (for

example, performance, security, availability, functionality, usability), those not discernible at run-time (modifiability, portability, reusability, inerrability, and testability), and those related to the architecture's intrinsic qualities (conceptual integrity, correctness, completeness, and buildability).

5.2. Quality Analysis and Evaluation Techniques

Various tools and techniques can help ensure a software design's quality.

- ◆ Software design reviews: informal or semiformal (group-based) techniques to verify and ensure the quality of design artifacts (architecture reviews, design reviews, and inspections; scenario-based techniques, requirements tracing). Software design reviews can also examine security, including performing vulnerability analysis. Installer, operator, and user aids (for example, manuals and help files) can be reviewed to ensure that they include security considerations.
- ◆ Static analysis: formal or semiformal static (non-executable) analysis that can be used to evaluate a design (for example, fault-tree analysis or automated cross-checking). Design vulnerability analysis (for example, static analysis for security weaknesses) can be performed if security is a concern. Formal design analysis uses mathematically based models that allow designers to predicate the behavior and validate the accuracy of software instead of having to rely entirely on non-assuring exhaustive testing. Formal design analysis can eliminate residual specification and design errors (caused by imprecision, ambiguity, and sometime splain mistakes).
- ◆ Simulation and prototyping: dynamic techniques to evaluate a design (performance simulation or feasibility prototype).

5.3. Measures

Measures can be used to assess or to quantitatively estimate various aspects of a software design's size, structure, or quality. Most measures that have been proposed generally depend on the approach used for producing the design. These measures are classified in two broad categories:

- ◆ Function-oriented (structured) design measures: the design's structure, obtained mostly through functional decomposition; generally represented as a structure chart (sometimes called a hierarchical diagram) on which various measures can be computed.
- ◆ Object-oriented design measures: the design's overall structure is often represented as a class diagram, on which various measures can be computed. Measures on the properties of each class's internal content can also be computed.

6. Software Design Notations Many notations and languages exist to represent software design artifacts. Some are used mainly to describe a design's structural organization, others to represent software behavior. Certain notations are used mostly during architectural design and others mainly during detailed design, although some notations can be used in both steps. In addition, some notations are used mostly in the context of specific methods. Note that software design is often accomplished using multiple notations: they are categorized into notations for describing the structural (static) view vs. the behavioral (dynamic) view.

6.1. Structural Descriptions (Static View)

The following notations, mostly (but not always) graphical, describe and represent the structural aspects of a software design: they describe the major components and how they are interconnected:

- ◆ Architecture description languages (ADLs): textual, often formal, languages used to describe software architecture in terms of components and connectors.
- ◆ Class and object diagrams: used to represent a set of classes (and objects) and their interrelationships.
- ◆ Component diagrams: used to represent a set of components ("physical and replaceable part[s] of a system that [conform] to and [provide] the realization of a set of interfaces") and their interrelationships.
- ◆ Class responsibility collaborator cards (CRCs): used to denote the names of components (class), their responsibilities, and their collaborating components' names.

- ◆ Deployment diagrams: used to represent a set of (physical) nodes and their interrelationships, and, thus, to model the physical aspects of a software. Usually, only certain deployed configurations are secure.
- ◆ Entity-relationship diagrams (ERDs): used to represent conceptual models of data stored in information systems.
- ◆ Interface description languages (IDLs): programming - like languages used to define the interfaces (names and types of exported operations) of software components.
- ◆ Jackson structure diagrams: used to describe the data structures in terms of sequence, selection, and iteration.
- ◆ Structure charts: used to describe the calling structure of programs (which module calls, and is called by, which other module).

6.2. Behavioral Descriptions (Dynamic View)

The following notations and languages, some graphical and some textual, are used to describe the dynamic behavior of software and components. Many of these notations are useful mostly, but not exclusively, during detailed design. Moreover, behavioral descriptions can include a rationale for why design will meet security requirements.

- ◆ Activity diagrams: used to show the control flow from activity (ongoing non-atomic execution within a state machine) to activity.
- ◆ Collaboration diagrams: used to show the interactions that occur among a group of objects; emphasis is on the objects, their links, and the messages they exchange on those links.
- ◆ Data flow diagrams (DFDs): used to show data flow among a set of processes. A data flow diagram provides "a description based on modeling the flow of information around a network of operational elements, which each element making use of or modifying the information flowing into that element". Data flows (and therefore possibly data-flow diagrams) are important to security as they offer possible paths for attack and disclosure of confidential information.
- ◆ Decision tables and diagrams: used to represent complex combinations of conditions and actions.
- ◆ Flowcharts and structured flowcharts: used to represent the flow of control and the associated actions to be performed.
- ◆ Sequence diagrams: used to show the interactions among a group of objects, with emphasis on the time-ordering of messages.
- ◆ State transition and statechart diagrams: used to show the control flow from state to state in a state machine.
- ◆ Formal specification languages: textual languages that use basic notions from mathematics (for example, logic, set, sequence) to rigorously and abstractly define software component interfaces and behavior, often in terms of pre- and post-conditions
- ◆ Pseudocode and program design languages (PDLs): structured-programming-like languages used to describe, generally at the detailed design stage, the behavior of a procedure or method.

7. Software Design Strategies and Methods There exist various general *strategies* to help guide the design process. In contrast with general strategies, *methods* are more specific in that they generally suggest and provide a set of notations to be used with the method, a description of the process to be used when following the method, and a set of guidelines in using the method. Such methods are useful as a means of transferring knowledge and as a common framework for teams of software engineers.

7.1. General Strategies

Some often-cited examples of general strategies useful in the design process include the divide-and-conquer and stepwise refinement strategies, top-down vs. bottom-up strategies, and strategies making use of heuristics, use of patterns and pattern languages, and use of an iterative and incremental approach.

7.2. Function-Oriented (Structured) Design

This is one of the classical methods of software design, where decomposition centers on identifying the major software functions and then elaborating and refining them in a top-down manner. Structured design is generally used after structured analysis, thus producing (among other things) data flow diagrams and associated

process descriptions. Researchers have proposed various strategies (for example, transformation analysis, transaction analysis) and heuristics (fan-in/fan-out, scope of effect vs. scope of control) to transform a DFD into a software architecture generally represented as a structure chart.

7.3. Object-Oriented Design

Numerous software design methods based on objects have been proposed. The field has evolved from the early object-oriented (OO) design of the mid-1980s (noun = object; verb = method; adjective = attribute), where inheritance and polymorphism play a key role, to the field of component-based design, where meta-information can be defined and accessed (through reflection, for example). Although OO design's roots stem from the concept of data abstraction, responsibility-driven design has also been proposed as an alternative approach to OO design.

7.4. Data-Structure-Centered Design

Data-structure-centered design starts from the data structures a program manipulates rather than from the function it performs. The software engineer first describes the input and output data structures (using Jackson's structure diagrams, for instance) and then develops the program's control structure based on these data structure diagrams. Various heuristics have been proposed to deal with special cases-for example, when there is a mismatch between the input and output structures.

7.5. Component-Based Design

A software component is an independent unit, having well-defined interfaces and dependencies that can be composed and deployed independently. Component-based design addresses issues related to providing, developing, and integrating such components in order to improve reuse. Reused and off-the-shelf software components should meet the same security requirements as new software. Trust management is a design concern; components treated as having a certain degree of trustworthiness cannot depend on less trustworthy components or services.

7.6. Other Methods

Agile methods propose to quickly implement an incremental basis by reducing emphasis on rigorous software requirement and design. Aspect-oriented design is a method which designs a software by using aspects to implement the cross-cutting concerns and extensions that are identified during the software requirements engineering process.

Service-oriented architecture is away to build distributed software using web service.

8. Software Design Tools They are used for design activities during the software development process. They assist designers in transforming software requirement specifications into software design artifacts. In detail, they implement part or whole of the following functions: to translate the requirements model into a design representation; to provide a notation for representing functional components and their interface; to implement heuristics refinement and partitioning; to provide guidelines for quality assessment.

In summary, a software design is a multi-faceted artifact produced by the design process and generally composed of relatively independent and orthogonal views.

Literature:

- 1.ISO/IEC/IEEE, ISO/IEC/IEEE998, 12207:2008: Information Technology -999 Software Life Cycle Processes, 2nd ed, 2008.
- 2.DeMarco T, The Paradox of Software Architecture and Design Stevens Prize Lecture, 1999
- 3.Budgen D., Software Design, 2nd ed., New York: Addison-Wesley, 2003
- 4.Sommerville I, Software Engineering 9th ed. New York: Addison-Wesley 2010
- 5.I 1016-2009 IEEE standard for Information Technology-Systems Design-Software Design Descriptions, ed, 2009.
- 6.Pressman R. , Software Engineering: A Practitioner's Approach 7th ed. The McGraw-Hill Companies, 2010.,
- 7.IEEE/ISO/IEC, IEEE/ISO/IEC Systems &Software Engineering Vocabulary, 1st ed. 2010

MATHEMATICS INDUSTRY ECONOMY – MICRO-FOUNDRY

Bushev St. PhD. assoc. prof. eng.
 Institute of Metal Science, Equipment and Technologies with Center for Hydro and Aerodynamics
 "Acad. Angel Balevski" – BAS, Sofia, Bulgaria
 stbushev@abv.bg

Abstract: This article presents fundamental results in mathematics and mathematical physics on the example of a theoretical model of structure formation in casting. Basic scientific results are innovations for all micro-foundries.

Keywords: FUNDAMENTAL RESULTS, MATHEMATICS & MATEMATICAL PHYSICS, INOVATIONS, MICRO-FOUNDRY

1. Introduction – Mathematics and economy

1.1 Mathematics

Definition of mathematics is by historical approach [1]: 1. Early definitions – Aristotle; 2. Greater abstraction and competing philosophical schools; 3. Definition in general reference works. Our opinion: mathematics is the science that takes care of its internal logic and never abandons not solved problems. Not resolved tasks often resolved after centuries.

In this work we present mathematics with it in our papers. The mathematical based of the casting is theory of heat conductivity – Stefan-Schwarz problem. This theory today is developing by modern mathematics and mathematical physics for investigate by computational physics to design new structure at phase transition.

Paper [2] presented the fundamental role of mathematics in thermodynamics. Other bright example for interaction between mathematics and physics is [3]. Today computational physics is a great part of investigations [7]. Multiscales modeling is introduced in [4 and 5]. At work with multiscale modeling must be render an account Gödel's theorems for precision of interaction between different mathematical methods.

For description of structure is use mathematical description in solidification zone introduce not only numerically of phase transition like area, but and descript and polycrystalline structure formation with maximum details. The first is mathematical theory of scattering for introduction driving force of crystallization [9]. Second is description polycrystalline structure formation by quantum mechanics: the equations of the molecular mechanics

$$\ddot{m}_i \ddot{r}_i = f_i \quad f_i = \partial U / \partial r_i, \quad (\text{MM})$$

$$-\hbar^2 \nabla^2 \psi(r) / 2m + V(r) = E \psi(r) \quad (\text{Schrödinger equation, 1, 2})$$

$$i\hbar \partial \psi(r,t) / \partial t = -\hbar^2 / 2m \partial \psi(r,r) / \partial r^2$$

where m , r and f_i – mass, coordinates and acting on atomic force derived from potential energy $U(r^N)$, where $r^N = (r_1, r_2, \dots, r_N)$ introduced full set of $3N$ coordinates of atoms; Planck's constant $-\hbar$; ψ - wave function, m – mass of the electron. The potential energy can introduce: interaction between not connection or connected atoms; the atoms and electrons building the crystal lattice and behavior of electrons are describes with Schrödinger's equation.

For this equations is used methods which introduced of micro-foundry applied in their practice by investment of mathematical results – software. In work [6] present term open innovation which introduced Henry Kembarou in 2003 paradigm that requires companies to use external ideas as well as internal to find advanced technology. For companies this is an open market approach science technological transfer "maximum speed" to market a new product.

On Fig. 1 is show schema of office for technological transfer (OTT) which subject is to develop a system for services of branch machine building particularly – micro-foundry. That system mast helps full innovation process. Micro-foundries have not many and innovation capacitance. The generation of an idea mast lead to a

reasoned decision with minimal risk. On Fig.1 is shown the schema of OTT

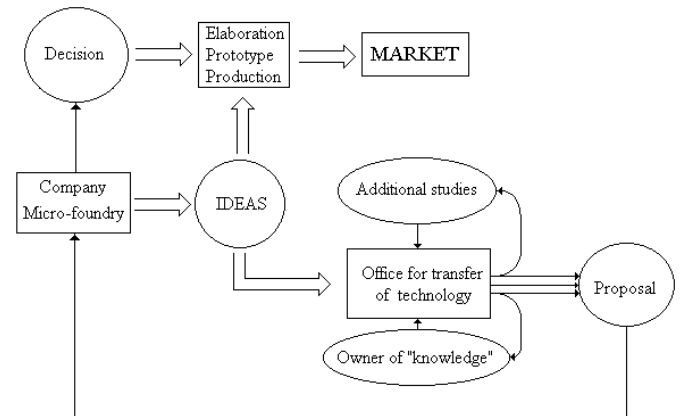


Fig.1 Schema of Offices transfer of technology and knowledge [6].

2. Micro-foundry – application of science and technology in casting practice

Fig. 2 presents the subject of foundry work: Fig. 2 a mold with cavity cast and Fig. 2 b machine for gas casting pressure

a) Aircraft Engine: (C) - Cast;
 (M=M₁+M₂+M₃+M₄) - Mould;
 boundary: W_{M/C}, Γ; - inlet.

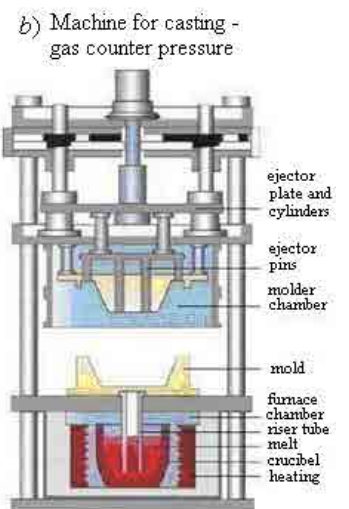
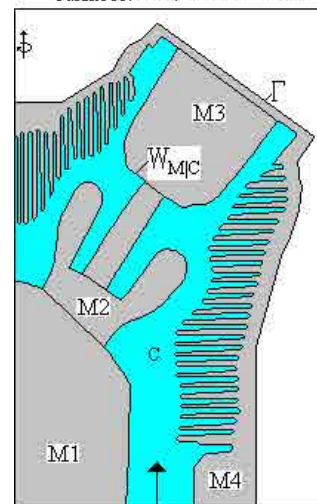


Fig.2 Casting technology.

3. Offices for science and technological transfer of branch machine building – micro-foundry

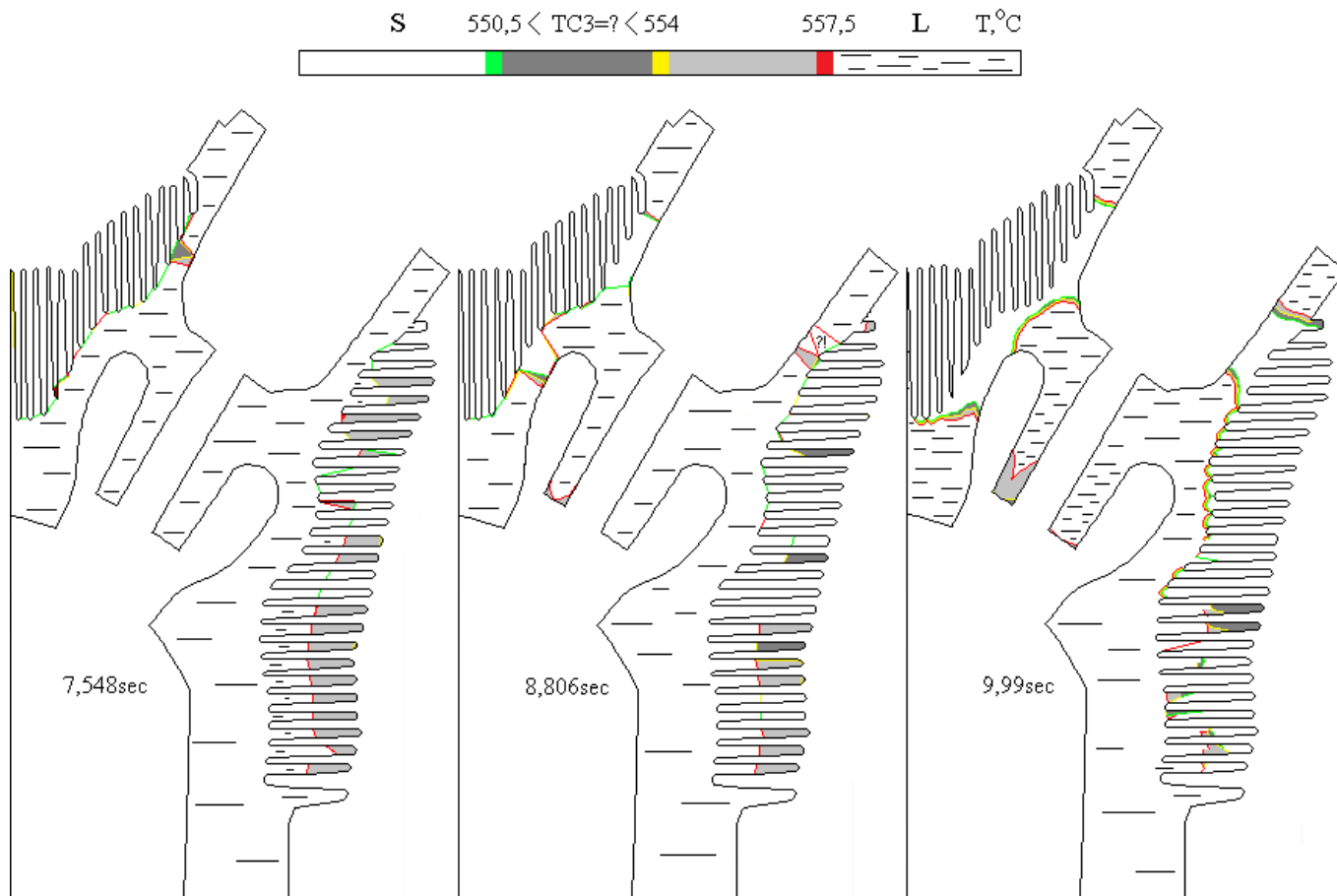
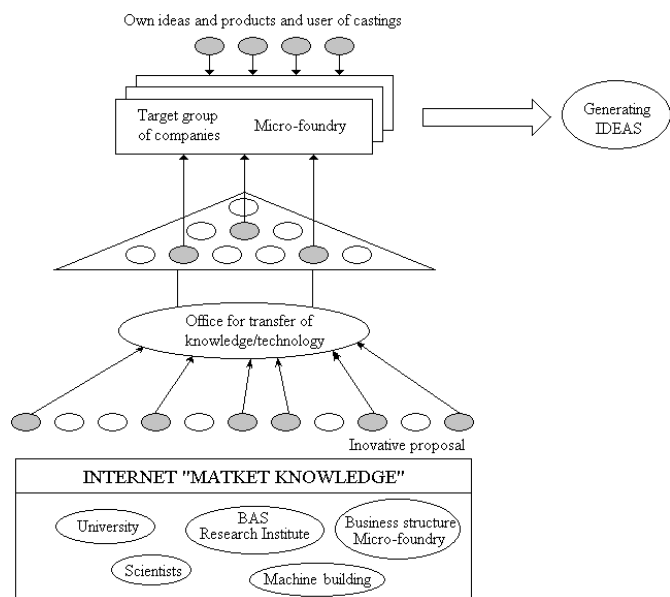


Fig. 1 Phase Transition: a) Fundamental states of the matter and different phase transition processes; b) Phase diagram a single component system [13]; c) thermodynamic diving force and crystallization of liquid [13]; d) Phase diagram of a second order quantum phase transition; Solidification process – zone of phase transition.

Thermodynamics system:
 Mathematical
 The nature

3. Conclusion
 Micro-foundry.

4. References

1. https://en.wikipedia.org/wiki/Definitions_of_mathematics
2. R. Clausius, Mechanical theory of heat, with its application to the steam-engine and to the physical properties of bodies, Jon Van Voorst, 1 Paternoster Row. MDCCCLXVII, London. <http://books.google.com>
3. I. Todorov, Einstein and Hilbert: The creation of general relativity, The world of physics, 1, 2014, 1-14. (In Bulgarian)
4. M. Tompa, Lectures, Dep. of Computer Science and Eng. FR-35, Univ. Washington, Seattle, Washington, U.S.A. 98195, 1991.
5. Weinan E, Principles of Multiscales Modeling, Cambridge University Press, UK, 2011, ISBN 978-1-107-09654-7
6. R. Georgiev, Open innovation – based of sustainable operational the offices for technological transfer, NTSM, 2012, Sofia, not publishing (In Bulgarian).
7. Uzi Landman, Materials by numbers: Computations as tools of discovery, PNAS, May 10, 2005, vol. 102, no. 19, 6671–6678.

THE PROBLEM OF OVERLAPPING PROJECT ACTIVITIES WITH INTERDEPENDENCY

Prof. Gurevich G., Prof. Keren B., Prof. Laslo Z.

Department of Industrial Engineering and Management – SCE-Shamoon College of Engineering, Beer Sheva, Israel

gregoryg@sce.ac.il, baruchke@sce.ac.il, zohar@sce.ac.il

Abstract: This paper analyzes a simple project with two activities. The activities can be executed in a serial mode (separately), in a parallel mode (overlapping), or in a mixed mode (partly in a serial mode and partly in a parallel mode). There is interdependence between the activities and the duration-budget tradeoffs functions of the activities are defined differently for each execution strategy. The paper presents a deterministic duration-budget tradeoff model that takes into account the interdependence between the activities in order to determine the optimal execution-mode and the budget distributions among the project activities. A stochastic extension of the proposed model is also considered. The presented analysis can help project managers and practitioners in choosing the optimal overlapping strategy for different objective functions and constraints.

Keywords: DURATION-BUDGET TRADEOFF, OVERLAPPING, INTERDEPENDENCE, TIME CONSTRAINT.

1. Introduction

There are three main techniques for project time compression: activity crashing, substitution and overlapping (Hazini et al. [1]). Crashing is a schedule compression technique in which cost and schedule tradeoffs are analyzed to determine how to optimize the best schedule compression for the least cost (Laslo and Gurevich [2]-[5], Laslo et al. [6]). Activity substitution involves the replacement of one activity or a sequence of activities in a series by other activities. Overlapping is a schedule compression technique in which activities that normally executed in sequence, are executed in parallel. Terwiesch and Loch [7] claimed that overlapping research and development activities are widely used to reduce project completion times. Dehghan et al. [8] restated that for a typical construction project, a number of overlapping strategies exist which can result a timesaving. The cost of these strategies varies significantly depending on the total rework and complexity they generate. Therefore, the best overlapping strategy that generates the required timesaving at a minimum cost should be found.

This paper analyzes a simple project with two activities. The activities can be executed separately, with overlapping (in a parallel mode), or in a mixed mode (partly separately and partly in a parallel mode). There is interdependence between the activities and the duration-budget tradeoff functions of the activities are defined differently if the activities are executed separately, in a parallel mode or in a mixed mode. The presented deterministic duration-budget tradeoff model takes into account the interdependence between the activities and helps to determine the optimal strategy for different objective functions and constraints. In particular, the model allows to determine: 1) the optimal execution-mode that minimizes the total project duration given that the budget of each activity is already allocated; 2) the optimal execution-mode and the budget distribution that minimize the total project duration, given a fixed total budget that should be optimally distributed among the activities; 3) the optimal execution-mode, the budget size and the budget distribution among the activities that minimize the total expenses, given the penalties/bonuses for a delay/early completion time; 4) the optimal execution-mode and the budget distribution that minimize the total budget for the project, given a constraint on the completion time of the project. A stochastic extension of the proposed model is also being considered. In the stochastic context, the activities durations are random variables where the expected values of the durations are results of the budget size that is invested in each activity

2. Model description

The *duration-budget tradeoff* functions for activities $i = 1, 2$ are defined differently for situations where the activities executed separately or jointly.

If the two activities are executed separately, then the *duration-budget tradeoff* functions for the first and second activities are defined by the following equation

$$\begin{aligned} t_1 &= f_1(b_1), \\ t_2 &= f_2(b_2), \end{aligned} \quad (1)$$

where, t_i is the i 's activity duration if both activities are executed in series, b_i is the budget allocated to activity i , $b_{iN} \leq b_i \leq b_{iC}$, b_{iN} is the known normal (minimal) budget that can be allocated to activity i , b_{iC} is the known crash (maximal) budget that can be allocated to the activity, $f_i(b_i)$ is the estimated (known) *duration-budget tradeoff*, a decreasing function that characterizes the duration of the i 's activity when both activities are executed in series. The end points of the function $f_i(b_i)$ are the normal (maximal) duration $f_i(b_{iN})$ corresponding to the known normal (minimal) budget b_{iN} , and the crash (minimal) duration, $f_i(b_{iC})$ corresponding to the known crash (maximal) budget b_{iC} , $f_i(b_{iC}) \leq f_i(b_i) \leq f_i(b_{iN})$, $i = 1, 2$.

If the two activities are executed in parallel, then the *duration-budget tradeoff* functions for the first and second activities are defined by the following equation

$$\begin{aligned} t_1^* &= f_1^*(b_1), \\ t_2^* &= f_2^*(b_2), \end{aligned} \quad (2)$$

where, t_i^* is the i 's activity duration if the two activities are executed in parallel, $f_i^*(b_i)$ is the estimated (known) *duration-budget tradeoff*, a decreasing function that characterizes the duration of the i 's activity if both activities are executed jointly. The end points of the *duration-budget tradeoff* function $f_i^*(b_i)$ are the normal (maximal) duration $f_i^*(b_{iN})$ corresponding to the known normal (minimal) budget b_{iN} , and the crash (minimal) duration, $f_i^*(b_{iC})$ corresponding to the known crash (maximal) budget b_{iC} , $f_i^*(b_{iC}) \leq f_i^*(b_i) \leq f_i^*(b_{iN})$, $i = 1, 2$.

The model assumes that the rate of execution of both activities is constant. Let x and y be decision variables that defined the portions of the first and the second activity, respectively, that are executed jointly, $0 \leq x = x(b_1, b_2) \leq 1$,

$0 \leq y = y(b_1, b_2) \leq 1$. Then, by (1)-(2), the total durations of the two activities are:

$$xt_1^* + (1-x)t_1 = xf_1^*(b_1) + (1-x)f_1(b_1), \quad (3)$$

$$yt_2^* + (1-y)t_2 = yf_2^*(b_2) + (1-y)f_2(b_2),$$

respectively. Moreover, since $xf_1^*(b_1) = yf_2^*(b_2)$, then by equation (3) the total duration of the project is

$$t = xf_1^*(b_1) + (1-x)f_1(b_1) + \left(1-x \frac{f_1^*(b_1)}{f_2^*(b_2)}\right) f_2(b_2). \quad (4)$$

3 Analysis of working strategies and budget distributions among the project activities

This section analyses the optimal working strategies and budget distributions among the project activities in the context of four different objective functions.

3.1. The optimal strategy that minimizes the total project duration given a fixed budget allocated to each activity

The considered problem is to minimize the total duration of the project, t , given the values of b_1 and b_2 , $b_{1N} \leq b_1 \leq b_{1C}$, $b_{2N} \leq b_2 \leq b_{2C}$. It means that the problem is to determine the value $x = x^*$ that minimizes the total duration of the project. Since $0 \leq x \leq 1$, $0 \leq y \leq 1$, then the optimal portion of overlapping x^* can be expressed by equation (4) as follows

$$x^* = \arg \min_{0 \leq x \leq \min\left\{1, \frac{f_2^*(b_2)}{f_1^*(b_1)}\right\}} \left\{ xf_1^*(b_1) + (1-x)f_1(b_1) + \left(1-x \frac{f_1^*(b_1)}{f_2^*(b_2)}\right) f_2(b_2) \right\}. \quad (5)$$

The following Proposition 1 presents the solutions x^* of equation (5).

Proposition 1. Given values of b_1 and b_2 ($b_{1N} \leq b_1 \leq b_{1C}$, $b_{2N} \leq b_2 \leq b_{2C}$), the solutions x^* of equation (5) are defined as follows.

If $f_1^*(b_1) \left(1 - \frac{f_2(b_2)}{f_2^*(b_2)}\right) - f_1(b_1) > 0$ then equation (5) has

the unique solution $x^* = 0$,

If $f_1^*(b_1) \left(1 - \frac{f_2(b_2)}{f_2^*(b_2)}\right) - f_1(b_1) < 0$ then equation (5) has the unique solution

$$x^* = \min \left\{ 1, \frac{f_2^*(b_2)}{f_1^*(b_1)} \right\} = \begin{cases} 1 & \text{if } f_2^*(b_2) \geq f_1^*(b_1) \\ \frac{f_2^*(b_2)}{f_1^*(b_1)} & \text{if } f_2^*(b_2) < f_1^*(b_1) \end{cases},$$

If $f_1^*(b_1) \left(1 - \frac{f_2(b_2)}{f_2^*(b_2)}\right) - f_1(b_1) = 0$ then each

$$x^* \in \left[0, \min \left\{ 1, \frac{f_2^*(b_2)}{f_1^*(b_1)} \right\} \right] \text{ is a solution of equation (5).}$$

3.2. The optimal strategy and budget distribution that minimize the total project duration given a fixed total budget for the project

Let b be an additional available budget that can be added to the normal (minimal) budget of the project's activities, $b_{1N} + b_{2N}$, $0 \leq b \leq (b_{1C} + b_{2C}) - (b_{1N} + b_{2N})$, and b_{ai} be an additional budget that can be added to the normal (minimal) budget of the i 's project activity $0 \leq b_{ai} \leq b_{iC} - b_{iN}$, $i = 1, 2$. That is, the budgets that can be allocated to the first and second project activities are $b_1 = b_{1N} + b_{a1}$, $b_2 = b_{2N} + b_{a2}$, respectively, where $b_{a2} = b - b_{a1}$. The considered problem is to minimize the total project duration, t , given the amount b of the additional budget. In other words, the problem is to determine values $b_{a1} = b_{a1}^*$ and $x = x^*$ of equation (4) such that

$$\begin{aligned} & \left(b_{a1}^*, x^* \right) \\ & = \arg \min_{(b_{a1}, x) \in A} \left\{ xf_1^*(b_{1N} + b_{a1}) + (1-x)f_1(b_{1N} + b_{a1}) + \left(1-x \frac{f_1^*(b_{1N} + b_{a1})}{f_2^*(b_{2N} + b - b_{a1})}\right) f_2(b_{2N} + b - b_{a1}) \right\}, \quad (6) \\ & A = \left\{ (b_{a1}, x) : 0 \leq b_{a1} \leq \min\{b, b_{1C} - b_{1N}\}, \right. \\ & \quad \left. 0 \leq x \leq \min \left\{ 1, \frac{f_2^*(b_2)}{f_1^*(b_1)} \right\} \right\}. \end{aligned}$$

Equation (6) is a standard mathematical programming problem of minimization of a function with two decision variables, b_{a1} and x .

3.3. The optimal strategy and the budget distribution that minimize the total project expenses given the penalties for a delay and the bonuses for earlier completion time

Let t_0 be a given agreed completion time of the project. The known function $g(t - t_0)$ defines penalties/bonuses for a delayed/earlier completion time. That is, $g(t - t_0) \geq 0$ if $t \geq t_0$, and $g(t - t_0) \leq 0$ if $t \leq t_0$. The total project expenses are defined as

$$c = b_1 + b_2 + g(t - t_0), \quad (7)$$

where $b_{iN} \leq b_i \leq b_{iC}$, $i = 1, 2$, $t = t(b_1, b_2, x)$ are defined by equation (4). The considered problem is to minimize the total project expenses C as defined by equation (7). Thus, the problem is to determine the values $b_i = b_i^*$, $i = 1, 2$, and $x = x^*$ such that

$$(b_1^*, b_2^*, x^*) = \arg \min_{(b_1, b_2, x) \in B} \{b_1 + b_2 + g(t - t_0)\}, \quad (8)$$

$$B = \left\{ (b_1, b_2, x) : b_{1N} \leq b_1 \leq b_{1C}, b_{2N} \leq b_2 \leq b_{2C}, \right. \\ \left. 0 \leq x \leq \min \left\{ 1, \frac{f_2^*(b_2)}{f_1^*(b_1)} \right\} \right\}.$$

Equation (8) is a standard mathematical programming problem of minimization of a function with three decision variables: b_1 , b_2 and x

$$(b_{iN} \leq b_i \leq b_{iC}, \quad i = 1, 2, \\ 0 \leq x \leq \min \{1, f_2^*(b_2) / f_1^*(b_1)\}).$$

3.4. The optimal strategy and budget distribution that minimize the total needed budget given a time constraint on the total duration

Assume a situation where there is a time constraint on the total duration of the project, $t \leq t_0$, where t_0 is a known value. The considered problem is to minimize the total budget, $b_1 + b_2$, subject to a given time constraint on the total duration, $t \leq t_0$, where t is defined by equation (4). Thus, the problem is to determine the values $b_i = b_i^*$, $i = 1, 2$, and $x = x^*$ such that

$$(b_1^*, b_2^*, x^*) = \arg \min_{(b_1, b_2, x) \in B} \{b_1 + b_2\} \quad (9)$$

$$s.t. \\ t \leq t_0,$$

where B is defined in equation (8). This is also a standard mathematical programming problem.

4. A stochastic extension of the model

In this section, the durations of the activities $i = 1, 2$ are assumed to be random variables. Similarly to the model presented in section 3, the *duration-budget tradeoff* functions for activities $i = 1, 2$ are defined differently when the activities are executed in a serial mode or in a parallel mode.

If the two activities are executed separately, then the *duration-budget tradeoff* functions for the first and the second activities are defined by the following equation

$$t_1 = f_1(b_1) + \varepsilon_1(b_1), \quad (10) \\ t_2 = f_2(b_2) + \varepsilon_2(b_2).$$

where, b_i , $f_i(b_i)$ are defined as in equation (1), $i = 1, 2$, $\varepsilon_1(b_1)$ and $\varepsilon_2(b_2)$ are independent random variables with zero expectations, $E(\varepsilon_1(b_1)) = E(\varepsilon_2(b_2)) = 0$.

If the two activities are executed jointly, then the *duration-budget tradeoff* functions for the first and the second activities are defined by the following equation

$$t_1^* = f_1^*(b_1) + \varepsilon_1^*(b_1), \quad (11) \\ t_2^* = f_2^*(b_2) + \varepsilon_2^*(b_2).$$

where, $f_i^*(b_i)$ is defined as in equation (2), $i = 1, 2$, $\varepsilon_1^*(b_1)$ and $\varepsilon_2^*(b_2)$ are independent random variables with zero expectations, $E(\varepsilon_1^*(b_1)) = E(\varepsilon_2^*(b_2)) = 0$.

The strategy for project execution in the stochastic case can be defined as follows. The two activities should be executed in parallel until a portion x of the first activity or a portion y of the second activity will be completed, where the variables $0 \leq x = x(b_1, b_2) \leq 1$ and $0 \leq y = y(b_1, b_2) \leq 1$ are decision variables. The rest of the activities should be executed in a serial mode. The rate of execution of both of activities is assumed to be constant. In this framework, the duration where both activities are executed in parallel, $\min\{xt_1^*, yt_2^*\}$, and the total duration of the

project, t , are random variables. Straightforwardly, by the law of total expectation, it can be shown that the expected value of the total duration of the project is

$$E(t) \\ = E \left(\left(\left(E(xt_1^* | xt_1^* \leq yt_2^*, t_2^*) + (1-x)E(t_1) \right) \right) \right. \\ \left. + \left(\left(1 - \frac{1}{t_2^*} E(xt_1^* | xt_1^* \leq yt_2^*, t_2^*) \right) E(t_2) \right) \right) \\ \left. \times P(xt_1^* \leq yt_2^* | t_2^*) \right) \\ + E \left(\left(\left(yt_2^* + (1-y)E(t_2) \right) \right) \right. \\ \left. + \left(\left(1 - yt_2^* E\left(\frac{1}{t_1^*} | xt_1^* > yt_2^*, t_2^*\right) \right) E(t_1) \right) \right) \\ \left. \times P(xt_1^* > yt_2^* | t_2^*) \right)$$

In a stochastic framework, equation (12) will be used instead of equation (1). Thus, the optimal strategies and the budget distribution among the project activities for the stochastic case can be analyzed in a similar way as was presented in section 3 for different objective functions.

5. Conclusions

In a real life projects have interdependency among their activities, and a parallel execution-mode may increase or decrease the activity duration and the total completion time of a project. We believe that the proposed analysis will help practitioners to select the optimal execution-mode, which is not trivial in the general case and can be a mixed one. Future research is needed to solve the stochastic problems for different distribution functions of project activities durations and to generalize the presented analysis for large projects with many activities.

6. References

1. Hazini, K., Dehghan, R. and Ruwanpura, J.Y. (2013). A heuristic method to determine optimum degree of activity accelerating and overlapping in schedule compression. *Canadian Journal of Civil Engineering*, 40(4), pp: 382-391.
2. Laslo, Z. and Gurevich, G. (2015). Planning and controlling projects under uncertainty. *American Journal of Operational Research*, 5(3), pp: 47-56.
3. Laslo, Z. and Gurevich, G. (2014). Enhancing project on time within budget performance by implementing proper control routines. *Management*, 72, pp: 53-69.
4. Laslo, Z. and Gurevich, G. (2013). PERT-type projects: time-cost tradeoffs under uncertainty. *Simulation: Transactions of the Society for Modeling and Simulation International*, 89(3), pp: 278-293.
5. Laslo, Z. and Gurevich, G. (2007). Minimal budget for activities chain with chance constrained lead-time. *International Journal of Production Economics*, 107(1), pp: 164-172.
6. Laslo, Z., Gurevich, G. and Keren, B. (2009). Economic distribution of budget among producers for fulfilling orders under delivery chance constraints. *International Journal of Production Economics*, 122(2), pp: 656-662.
7. Terwiesch, C. and Loch, C.H. (1999). Measuring the effectiveness of overlapping development activities. *Management science*, 45(4), pp: 455-465.
8. Dehghan, R., Hazini, K. and Ruwanpura, J. (2015). Optimization of overlapping activities in the design phase of construction projects. *Automation in Construction*, 59, pp: 81-95.

SUMMARY OF INNOVATION MODELS ON A COMPANY LEVEL – CREATING A FRAMEWORK FOR AN INNOVATION MODEL THAT WILL INCREASE A COMPANY’S INNOVATION ACTIVITY

M.Sc. Stefanovska Ceravolo LJ.¹, Prof. PhD. Polenakovikj R.², Prof. PhD Dzidrov M.¹
 Faculty of Mechanical Engineering – University “Goce Delcev” in Stip, Republic of Macedonia¹
 Faculty of Mechanical Engineering – University “Ss.Cyril and Methodius” in Skopje, Republic of Macedonia²
 ljubica.stefanovska@ugd.edu.mk

Abstract: There are six known and generally accepted generations of innovation models. Innovation models transform from simple, linear models, to integrated and networking models that are dynamic and interactive. Each generation of innovation models is presented in this paper with their characteristics as well as drawbacks. The main goal of this paper is to show the transformation path of innovation models and create a framework for a new innovation model on a company level, that could be used by companies to increase their innovative activity and performance. Innovation models define the innovation process and its phases. The framework for the new innovation model includes feedback that was lacking in the first and the second generation of innovation models, but is included in the other generations. It also includes integrated and networking activities which are a characteristic of the third and fourth generation of innovation models. Another component of the model is the usage of information and communications technology (ICT) to facilitate the process of innovation, which is one of the characteristic of the fifth generation of innovation models. It uses a process approach and is based on the open innovation model, which is the signature model from the sixth generation of innovation models and best represents the complex system and characteristic of innovation. The model is supposed to help companies generate innovative ideas and select them through a predetermined process with four main components that act as control points. The purpose of this model is to create a continuous culture for innovation and to set up official procedures. These will help companies to accomplish their innovative ideas and activities.

Keywords: INNOVATION, INNOVATION MODELS, OPEN INNOVATION, TECHNOLOGICAL INNOVATION, INNOVATION PROCESS.

1. Introduction

Innovation models are being used so that companies can manage their innovation processes which have evolved tremendously in the last few decades of the XX century. Companies can adopt an existing model, or they can create their own [1]. By having an innovation model, it is easier to manage the order in which innovation activities happen. It also helps with determining the resources and responsibilities for every stage of the process as well as deciding which methods and tools companies will use. Innovation as a process has a very dynamic character, and the models of innovation have transformed throughout the years. Innovation models can be on a company level or a national level (such as National Innovation Systems – NIS) and can also be adopted and used by a region, an economy etc. In this paper we will focus on the company level innovation models. Based on the main characteristics of the different generations of innovation models, we are suggesting a framework for an innovation model that can be highly applicable to all company sizes, whose main goal is to increase the innovation activity and increase a company’s innovation performance.

2. Innovation models and their characteristics

Currently there are six known generations of innovation models, although a seventh generation of innovation models is mentioned by Kotsemir et al., that has “emerged”, but is “not formed yet” [2]. Rothwell’s five generations of innovation models give a historical perspective of innovations management that shows how innovation models have transformed from linear to complex interactive models [3]. The approach to innovation management Rothwell gives in his classification relates to the evolution of organizations, the strategies of innovations management under various socio-economic and political circumstances and doesn’t include the substantive development of the innovation models themselves [4]. Rothwell’s typology is based on models of innovation on a company level.

Another typology of innovation models is presented by Marinova and Phillimore where they present six generations of innovation models [5] and for their classification they use

technological models that apply to the overall economy, plus they give a theoretical background of the generations of the innovation models, as well as their positive and negative sides [6].

Table 1 shows the generations of innovation models by Rothwell [7] and Marinova & Phillimore [8].

Table 1. Generations of innovation models, author’s adaptation of Rothwell (1992) and Marinova & Phillimore (2003)

Generation	Period	Rothwell	Marinova & Phillimore
1	1950’s – mid 1960’s	Technology push model	The black box model
2	Mid 1960’s – early 1970’s	Market pull model	Linear models (technology push – need pull)
3	Early 1970’s – mid 1980’s	Interactive or Coupling model	Interactive models (coupling and integrated models)
4	Early 1980’s – early 1990’s	Integrated innovation process (parallel development)	Models of innovation systems (networks and national innovations system)
5	1990’s	SIN (Systems integration and Networking Model)	Evolutionary models
6			Innovation milieu

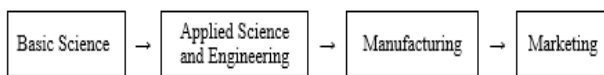
The model of *Innovation milieu* is considered to be a networking model that applies on a national level. On a company level though, the model of *Open Innovation* is the sixth generation model of innovation [9]. The father of the *open innovation model* is Henry W. Chesbrough, who has introduced this concept stating that innovation has become an increasingly open process thanks to a growing division of labor [10]. Therefore, we will present the six generations of models and their main phases and characteristics, as well as their drawbacks.

We will start with the *first generation of innovation models* and the famous *linear model of innovation (technology push)*. The main phases of this type of models are: 1) basic science/fundamental

research; 2) design and engineering; 3) manufacturing; 4) marketing and 5) sales [11,12]. This is a period where a lot of resources were put towards the R&D in companies, because it was believed that the more R&D is done, then more new products will be out. This pushed innovations forward, but did not give enough attention to the transformation process of existing products [13] or the needs of the market place and the consumers [14].

The second generation of innovation models is not much different from the first one. Both lack feedback loops, but the second one recognizes the fact that including the market/consumer needs will help drive performance and will be a source of ideas for new and better products/services [15]. Therefore, the second generation linear model of innovation is called the *linear model of innovation (market pull/demand pull)*. Both models are shown in **Figure 1** and these are the technology push and need pull models suggested by Rothwell.

“Technology-push” model:



“Need-pull” model:

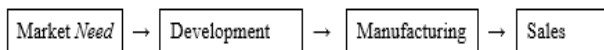


Fig. 1. Rothwell’s Diagram (source: Godin, 2013)

The first and second generation of innovation models have predetermined phases with a consecutive nature (as shown on **Figure 1**) and are both still being used today, with minor modifications such as adding control elements between each phase to approve the transitioning from one phase to another, and also to better the decision process just like the *stage-gate model*. This model was predominantly used by NASA in the 1960’s while trying to find creative innovative ideas to send a man on the Moon. This model, further simplified and suggested by Cooper [16] consists of five relevant phases or stages (as shown on **Figure 2**), and the added controlling elements here are *the gates* positioned after each phase. Their function is to follow the fulfillment of strict and predetermined criteria before we move onto the next stage [17]. Many other companies have adopted and used, or are still using, this model [18].

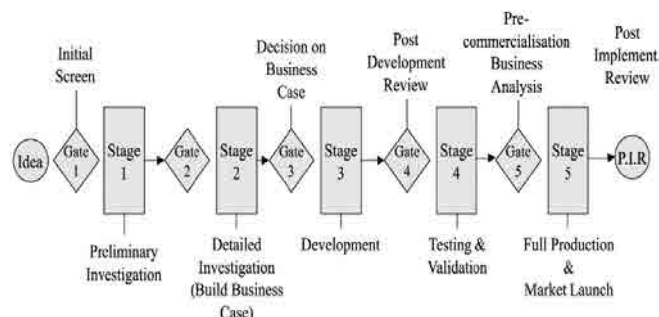


Fig. 2. Cooper’s Stage Gate Model (Source: Cooper, 1994)

The third generation of innovation models differ from the first and second significantly. These models are given the name *Interactive models* as a result of recognizing the interaction between elements in the innovation process which is a key for innovation’s success. The technology push and market pull models are “coupled” in this generation which implies suppliers and customers to be closely “coupled” in product development teams [19]. The models include interaction and feedback between phases such as the

marketing research and the other elements in the linear process [20], but could not differentiate the need from the demand. *The Coupling model of Mayers & Marquis* (as shown in **Figure 3** [21]) is a third generation innovation model, where the innovation activities are divided in subcategories under each phase, and all of them are interacting [22].

The fourth generation of innovation models corresponds to the Japanese perception of the innovation process and it was the answer to the need of replacing the linear model with a different model that can reflect the complex innovation process [23]. The models from this generation consist of the basic stages of the linear models of innovations, enriched by many feedback loops and interaction between the stages, as well as a validation of the knowledge gained in the innovation process [24].

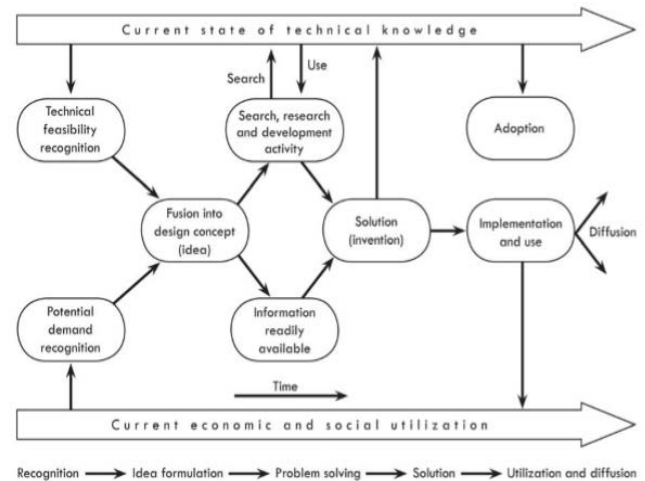


Fig. 3. The Myers and Marquis Coupling Model from 1969 (source Godin, 2013)

These models are also functionally integrated innovation models and they achieved integrating the suppliers, customers and partners in the development process [25]. On **Figure 4** is the *Chain-Linked Model*, developed by Rosenberg and Kline (1986).

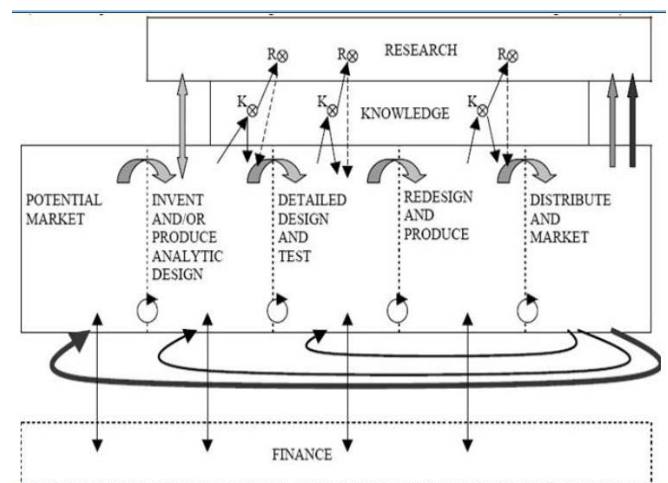


Fig. 4. The Chain-Linked Model of Innovation (Rosenberg and Kline, 1986) Source: www.uis.unesco.org.

After seeing a trend of cutting down on R&D costs companies had to network and find different ways to proceed with their innovative activities [26]. Information systems became the next big thing and started being incorporated into the companies work, especially in process automation and in expediting the communications inside a company’s network [27]. Therefore, the different activities within the innovation process became even more integrated and could occur simultaneously, with feedback loops. We

also notice a trend of overlapping functions. This is when the *fifth generation of innovation models* appeared. Rothwell's *SIN (Systems Integration and Networking)* model as a fifth generation innovation model incorporates the higher integration inside companies as well as with the outside entities such as suppliers, consumers, universities and authorities [28].

Introduced by Chesbrough, *The Open Innovation Model* (Figure 5) underlines idea management not just within the organizations, but also with other organizations. R&D is being done by outside partners, if it is not possible to be handled by the company itself, and ideas can occur while developing a new product/service which can change the course of the process. This model promotes using outside knowledge, such as suppliers, competition, entrepreneurs, scientists etc. [29].

The open innovation process can be 1) the *outside in process*; 2) the *inside out process*; and 3) the *coupling process* [30] and innovative ideas are introduced by outside sources such as universities, research centers, suppliers, competition, government bodies and consumers [31]. There are four main phases of this innovation model: 1) *research*; 2) *development*; 3) *manufacturing*; and 4) *marketing*, coupled with other processes and entities with an interactive nature [36]. R&D in this model is taken over by publicly funded research centers or universities where ideas are chosen through a highly competitive selection process which promotes transparency of innovation activities.

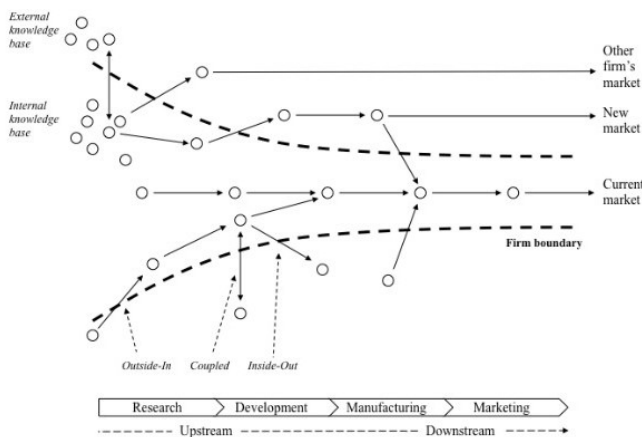


Fig. 5. The Open Innovation Model (Chesbrough, 2014)

Such models have been implemented in large companies, but there are also findings that open innovation models have been used in SME's as well, primarily for market related motives, such as meeting customer demands and keeping up with competitors where the biggest challenges lie in organizational and cultural issues as a consequence from dealing with increased external contacts [32].

3. Discussion

What we have learned from the six generations of innovation models is that a good innovation model has to have *predetermined phases*, *feedback loops*, large capability for *interaction* and *integration*, but also to be *knowledge based*, able to use outside knowledge, endorse knowledge gain and maintain the knowledge level in the company through achieving a continuous learning culture. Because the feedback loops were lacking in the first and second generation of innovation models, and customer's feedback is an essential element of innovation, we consider them as a part of every stage of the innovation process. Another element for a successful innovation process is *networking*, which will help companies of all sizes, not just the large ones that can afford their own R&D, to be able to innovate and enter new markets. This will also help in the effort of *knowing the competition* and keep in tune with the technological advances. *Identifying new sources* of ideas is crucial for generating innovative ideas, that has been used for the

first time in the second generation of innovation models, where market pull became the main source of ideas.

Planning a *reliable and safe funneling of ideas* and their distribution will encourage innovative minds to take part of the process and share their ideas and knowledge. The *selection process* of innovative ideas should be done by strict criteria and very carefully, and the model should be able to know whether it is *the right time* for introducing a certain innovation on the market or not. This should be enabled by using *marketing, legal, economical and development component* as a part of the process, where the marketing component can determine whether an idea can be marketable or not, the legal component will deal with the patenting potential of the innovative idea that can be an additional source of income and potential success, the economic component will be able to say how economically feasible the new idea is and whether we can use outside R&D facilities or other entities to help in the process; and the development component the actual R&D of the idea before bringing it to market and getting to the *realization and diffusion* stages.

4. Conclusion

The transformation process of the innovation models show that innovation is of a changing nature and very complexed. In order to suggest a new model that can help companies innovate more in regions with a low innovation activity trend, we need to take in consideration that no innovation can happen if the *company culture* doesn't enable this itself. For companies to become more innovative, they need to be *ready for change* and to have set up mechanisms that will support the process.

We can state that in order to have an innovation model that could be widely applicable to different types and sizes of companies, the model itself should be of a simple and maybe with a certain linear character, but with enough details that are going to clearly describe the innovation process. The main phases of the innovation model should be marketing, legal, economic, development, realization and diffusion phase, integrated with feedback loops, and potentially modified with other predetermined phases. It should include measures and tools for evaluation of feedback. The model should also be knowledge based, easy to adapt to a networking environment, handle interaction, know the competition and easily identify new sources of ideas that will be funneled through a predetermined channel. Achieving a continuous learning culture should be an integrated part of the model. As a beginning of the innovation process we can say that generation of ideas is the most important part, as well as planning a reliable and safe funneling and distribution of the same ideas.

5. References

- [1] Jovanoski, D., Innovations management, Skopje, University "Ss. Cyril and Methodius", Faculty of Mechanical engineering, 2012 (Jovanoski, D.)
- [2] Kotsemir, M.N., D. Meissner, Conceptualizing the innovation process—trends and outlook. Higher School of Economics Research Paper No. WP BPR, 10, 2013 (Kotsemir, M.N., D. Meissner)
- [3] Rothwell, R., Zegveld, W., Innovation and the small and medium sized firm, University of Illinois at Urbana-Champaign's Academy for Entrepreneurial Leadership Historical Research Reference in Entrepreneurship, 1982 (Rothwell, R., Zegveld, W.)
- [4] Kotsemir, M. N., A. Abroskin, D. Meissner: Innovation concepts and typology—an evolutionary discussion. Higher School of Economics Research Paper No. WP BRP. 2013, Feb 20;5. (Kotsemir, M.N., A. Abroskin, D. Meissner)
- [5,6] Marinova, D., Phillimore, J. Models of innovation, The international handbook on innovation, Elsevier, 2003, pp. 44-53 (Marinova, D., Phillimore D.)

- [7] Rothwell, R., Towards the Fifth-generation Innovation Process-International Marketing Review, Vol. 11 Iss: 1, 1994, pp.7 – 31 (Rothwell, R.)
- [8] same as [5,6]
- [9] same as [5,6]
- [10] Chesbrough, H. W., Why companies should have open business models - MIT Sloan management review, 48(2), 22, 2007 (Chesbrough, H. W.)
- [11] Godin, B., The Linear model of innovation the historical construction of an analytical framework - Science, Technology & Human Values, 31(6), 2006, pp.639-667. (Godin, B.)
- [12] Le Corre, A., Mischke, G., The innovation game: a new approach to innovation management and R&D, Springer, 2002 (Le Corre, A., Mischke, G.)
- [13] Carter, C. F., Williams, B. R., Industry and technical progress, 1957 (Carter, C. F., Williams, B. R.)
- [14] Rothwell, R., H. Wissema, Technology, culture and public policy - Technovation, 4(2), 1986, pp. 91-115 (Rothwell, R., H. Wissema)
- [15] Hughes, D. G., D. C. Chafin, Turning new product development into a continuous learning process - Journal of Product Innovation Management, 13(2), 1996, pp. 89-104 (Hughes, D.G., D.C.Chafin)
- [16] same as [11]
- [17] Cooper, R. G., E. J. Kleinschmidt, Stage-gate process for new product success - Innovation Management U 3 (2001): 2001 (Cooper, R.G., E. J. Kleinschmidt)
- [18] Cooper, R. G., S. J. Edgett, E. J. Kleinschmidt, Optimizing the stage-gate process: what best-practice companies do — I - Research-Technology Management, 45(5), 2002, pp.21-27. (Cooper, R. G., S. J. Edgett, E. J. Kleinschmidt)
- [19] Nicolov, M., Badulescu, A. D., Different types of innovation modeling – Annals of DAAAM of 2012 and Proceedings of 23rd DAAAM International Symposium, Volume 23, No.1, Vienna, Austria, 2012, pp. 1071-1074 (Nicolov, M., Badulescu, A. D.)
- [20] Hobday, M, Firm-level innovation models: perspectives on research in developed and developing countries - Technology Analysis & Strategic Management, 17(2), 2005, pp. 121-146 (Hobday, M.)
- [21] Godin, B., J. P. Lane, Pushes and Pulls Hi (S) tory of the Demand Pull Model of Innovation - Science, Technology & Human Values, 38(5), 2013, pp.621-654. (Godin, B. J., J. P. Lane)
- [22] same as [5,6]
- [23] Mahdjoubi, D., The Linear Model Of Technological Innovation: Background and Taxonomy, UTexas working paper, 1997 (Mahdjoubi, D.)
- [24] Ryan, C. D., P. W. Phillips, Knowledge management in advanced technology industries: an examination of international agricultural biotechnology clusters - Environment and Planning C, Government and Policy, 22(2), 2004, pp. 217-232 (Ryan, C. D., P. W. Phillips)
- [25] same as [19]
- [26] same as [20]
- [27] Gabison, G., Pesole, A., An Overview of Models of Distributed Innovation. Open Innovation, User Innovation, and Social Innovation. No. JRC93533, Institute for Prospective and Technological Studies, Joint Research Centre, 2014 (Ganbison, G., Pesole, A.)
- [28] same as [20]
- [29] same as [27]
- [30] Enkel, E. O. Gassmann, H. Chesbrough: Open R&D and open innovation: exploring the phenomenon - *R&D Management*, 39.4, 2009, pp. 311–316. (Enkel, E., O. Gassmann, H., Chesbrough)
- [31] same as [27]
- [32] Van de Vrande, V., J. P. De Jong, W. Vanhaverbeke, M. De Rochemont, Open innovation in SMEs: Trends, motives and management challenges – Technovation, 29(6), 2009, pp. 423-437. (Van de Vrande, V., J. P. De Jong, W. Vanhaverbeke, M. De Rochemont)

TOP INNOVATION IN MANAGEMENT OF AGRICULTURAL ACTIVITIES (EFFECTIVE BIOLOGICAL AGRICULTURE UNDER IRRIGATION AND PROTECTING THE ENVIRONMENT)

НОВШЕСТВО В УПРАВЛЕНИИ СЕЛЬСКОГО ХОЗЯЙСТВА

Prof. Dr. Christov I., Ph.D. & D.Sc.

Poushkarov Institute for Soil Science, Agrotechnology and Plant Protection - Sofia, Bulgaria
E-mail: ichtistow@gmail.com

Abstract/Резюме. The report deals with the perspectives for developing ecologically based biological agriculture in Bulgaria, the European Union and the other countries. Innovative technology (for computerized monitoring the soil water deficit and scheduling the irrigation) replaces the periodical local (point) measurements of soil moisture. Its application helps to be realized appropriate energy level of soil moisture through ecologically accepted watering technique in each agricultural crop field. It ensures to be obtained the scientifically planned amount and quality of crop yield, saving over ten years on average 30 % of irrigation water and one third of nutrients added for plants.

KEY WORDS: IRRIGATION, DECISION SUPPORT SYSTEM, NEW INDEX FOR ESTIMATING WATER STATUS.

1. Introduction/Введение

The development of agriculture under irrigation has to be accomplished on the new eco-biological scientific basis (Christov, 1989, 2008abcd), which was accepted by world leading scientists in USA, RF, etc. Technology based on it should be widely applied, according to the European requirements.

The scientific progress in biophysics of plant populations, soil and atmosphere physics, and ecology created actual prerequisites and practical possibilities for easy current taking into account the crop physiological features and ecological requirements when growing cultural plants in numerous agricultural fields (agroecosystems) for the first time in world.

New complex scientific basis is developed and tested under field conditions during a period of 30 years. Computerized ecological technology based on it, which has to be put into practices of biological agriculture under irrigation, is created (Christov, 1992, 2004 and 2012).

The basis applies and links the separate top scientific and technological achievements developed in UK, USA, Japan, Ukraine and Bulgaria. For the first time in the world, two Bulgarian High Scientific Attainments, which are necessary for the universal scientific basis, are included in it.

The complex innovation system (Fig. 1) practically ensures the necessary coordination between the plant physiological and the ecological requirements.

2. Prerequisites and means for solving the problem/Предпосылки и средства для решение проблемы

2.1. Plant Physiological features. For the first time in the world agricultural science and practice, the physiological processes in cultural plants, which concern the water and nutrients, are

practically taken into account (Christov, 2004). These processes are as follows.

1. The gradual decrease in soil moisture from field capacity (FC) to permanent wilting point (PWP) causes irreversible physiological processes with increasing intensity in the plant organism. For example, the established dependence of the losses, ΔY_{ec} (%), of maize grain yield on the drop, ΔL_{ec} ($J^{1/2}/kg^{1/2}$), of energy level of soil moisture at extreme-critical stage of ontogenesis only is shown in Fig. 2.

2. The degree of irreversible damage on plant is different under the same decrease in moisture of one and the same soil at separate stages of plant development (ontogenesis).

3. The maximal physiological damages at all stages are accumulated. They irreversibly limit the amount and quality of production independently on the next increase in soil moisture, which is caused by watering or precipitation (Fig. 3).

4. The irreversible physiological defeat depends on the energy condition of moisture in soil. This condition corresponds to different values of moisture in various soil textures.

2.2. Ecological requirements. In managing the agroecosystems, the ecological requirements are the following.

A. Agricultural activities must be implemented in ecologically-accepted form, protecting the environment (underground water, surface reservoirs, soil and atmosphere) from pollution.

B. Precise current estimation of the net norm of watering must takes into account the moment values of: depth of root layer of soil, water deficit in this layer, and water-retention capacity of each genetic horizon of soil, which on the day of watering is in the frame of the root zone.

These requirements can be introduced after putting into irrigation practices the top attainments aggregated in the new ecological technology. This will significantly precise the calculation of net

norm of watering. It will reduce or remove the amount of water, which causes the pollution by bearing pollutants (soluble nutrients for plants) to near underground water layers and to surface reservoirs located near the irrigated fields.

C. Appropriate watering technique, preventing the destroying and taking out of the soil by irrigation water through must be applied. The physical properties of soil and relief must be taken into account when controlling the watering process.

D. When applying the precisely determined watering norm, we must form the new water supply only in root layer on the determined day of watering. The watering norm must compensate only the moisture deficit in root layer under minimized loss of water.

E. Decreasing the losses of irrigation water, energy (electrical and from fuels), plant nutrients and human labour is possible to be reached implementing the irrigation schedule currently established through the offered technology.

3. Results and discussion/Результаты и обсуждение

Applying the technology under the extremely changing meteorological conditions over many years, we established the dependence of the amount of maize (H-708) yield on the soil water status estimated by us through the new biophysical index L of energy levels of soil moisture. The data on yield obtained under irrigation and non-irrigation are described through the equation:

$$(1) \quad Y = 19.45 - 0.55L$$

or in general form

$$(2) \quad Y = A - B L,$$

where: Y is the mass of grain yield (t/ha); L – the biophysical index ($J^{1/2}/kg^{1/2}$) of water status in root zone; A and B – the coefficients specifying the crop. The established correlation coefficient is equal to $R = -0.980$.

4. Conclusion/Заключение

The ecotechnology for current decisions during the growing season applies new estimation index of soil water status for the first time in agricultural sciences and practice. It is based on physical laws and biological regularities. No simulation models are used in the technology. It applies the complete set of current meteorological data for the current growing season.

The technology replaces the periodic measuring of soil moisture applying local (point) methods, which are not ensuring good representative data on soil moisture for the large field in agriculture. The application of point methods are consuming much human labour and time, and can not be successfully used for the enormous number of rural fields. The ecologically based

agriculture is perspective only under conditions of applying this innovative technology. Its application will help to create and keep appropriate energy level of soil moisture for the first time in many large crop fields under different meteorological conditions.

This technology is energy-saving, water-saving and ensures ecologically accepted management of soil water status. Its applying ensures the planned amount of yield and the determination of needed nutrients.

Its wide application helps to protect the environment and develop sustainable agriculture. It ensures effective control on the pollution of lakes, rivers, dams and underground water, which is caused by the applied traditional agricultural activities.

Application of the ecotechnology created the possibility to obtain each year **12 t/ha maize grain** (hybrid H-708) under the conditions of Calcareous Chernozem soil (near Lom, Bulgaria) during the period of 8 years (1981-1988), under extremely different meteorological conditions, saving **on average 30 % of the irrigation norm** compared to that recommended by the project schedule of irrigation for this crop in the region. The ecotechnology represents a great interest for buying by the farmers in the European Union and abroad, after transforming it in friendly for farmers and specialists **universal market system for managing**.

5. Literature/Литература

- Christov, I. Theoretical Basis for Crop Water Management. *International Agricultural Physics*, **5**, (3-4), 1989, 261-268.
- Christov, I. 1992. Energy Levels of Soil Moisture and Biolproductivity. *International Agricultural Physics*, **6**(1-2), 89-94.
- Christov, I. D. 2004. Estimation of Agroecosystem Water Status and Formation of Plant Water Supply in Soils. Monograph, Series Ecology, PublishScieSet-Eco, Sofia, p. 216, ISBN 954-749-044-3.
- Christov, I. 2008a. Management of Agroecosystem Water Status. Part 1. New Complex Scientific Base. *J. of Balkan Ecology*, **11**(1), 5-22.
- Christov, I. 2008b. Management of Agroecosystem Water Status. Part 2. Organization of Decision Support System (DSS) Application and Advantages. *Journal of Balkan Ecology*, **11**(2), 137-148.
- Christov, I. 2008c. Management of Agroecosystem Water Status. Part 3. Adequacy of Decision Support System (DSS). *J. of Balkan Ecology*, **11**(3), 229-240.
- Christov, I. 2008d. Management of Agroecosystem Water Status. Part 4. Relationships among Soil Moisture Energy Level, Soil Water Properties and Biological Features of Crop. *J. of Balkan Ecology*, **11**(4), 341-350.
- Christov, I. Monitoring and Management of Agroecosystem Water Status for Protecting Environment and Establishing Sustainable Agriculture. PublishScieSet-Eco, Sofia, 2012. p. 262, ISBN 978-954-749-098.

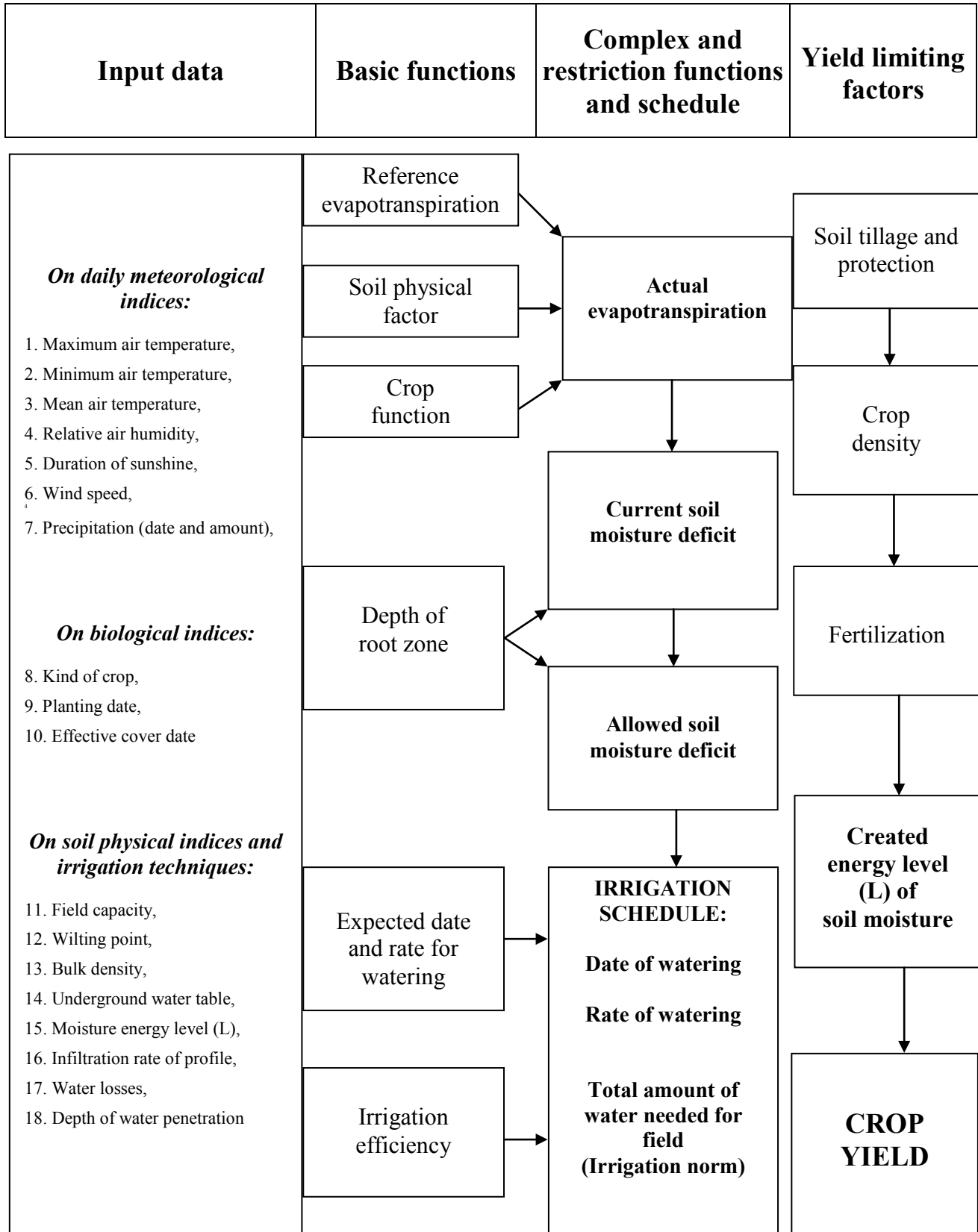


Fig. 1. Scheme of the Decision support system (DSS) for agroecosystem water status management

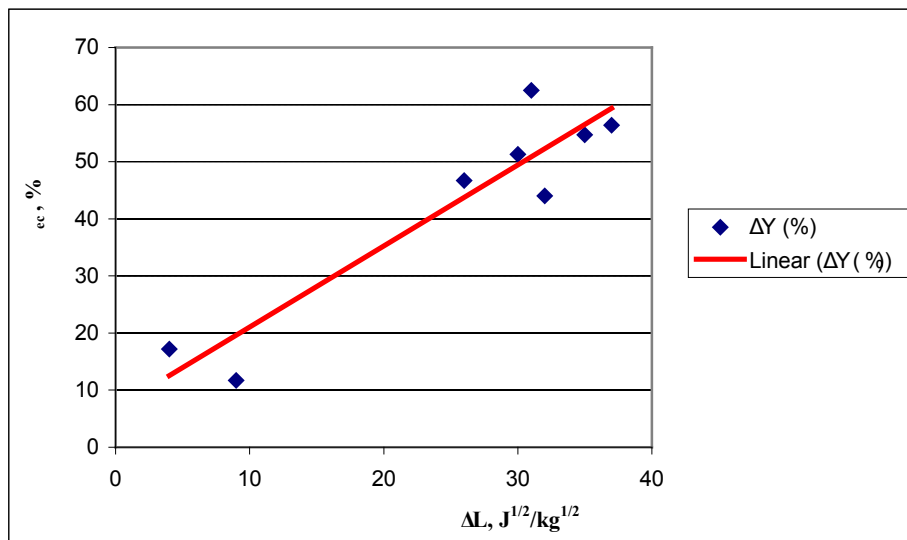


Fig. 2. Dependence of the losses, ΔY_{ec} (%), of maize grain yield on the drop, ΔL_{ec} ($J^{1/2}/kg^{1/2}$), of energy level of soil moisture under field conditions at extreme-critical stage of ontogenesis only (correlation coefficient is $R = 0.95$; equation is $\Delta Y_{ec} = 2.217 + 1.567 \Delta L$)

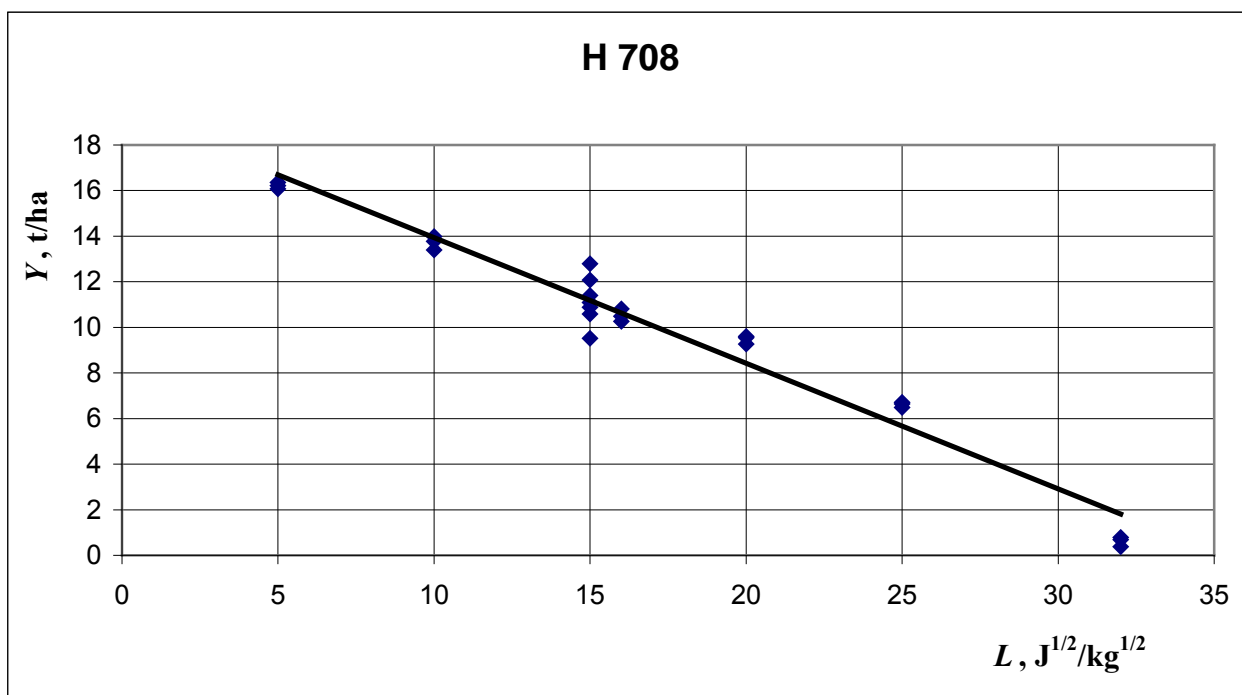


Fig. 3. Dependence of yield Y , t/ha, of maize grain (obtained at appropriate N , P and K nutrient rates determined through the DSS) on the integral index L , $J^{0.5}/kg^{0.5}$ (correlation coefficient $R = 0.98$; equation is $Y = -0.55L + 19.45$)

AN APPROACH TOWARDS PLANNING OF ELECTRIC VEHICLES CHARGING INFRASTRUCTURE BASED ON VEHICLE AND TRANSPORT STRUCTURE

M-r Stevan Kjosevski, dipl. mech. engineer, PhD student, Prof. d-r Atanas Kochov, dipl. mech. Engineer, Doc. d-r Aleksandar Kostikj, dipl. mech. Engineer, University "Ss. Cyril and Methodius" - Faculty of Mechanical Engineering – Skopje, Republic of Macedonia

Abstract – *Electrical vehicles are in a new phase of development and utilisation. It has been a long time before such initiatives have taken place. In the meantime the transport as a whole (vehicles, roads, traffic, etc.) has been significantly changed. As expected the main role in this process globally, and regionally is taken by the biggest economies and companies. Besides the environmental priorities, the nature of transport which does not recognise borders enforces smaller economies and countries to adopt their policies in this area, and take chances of the development. This seems to be very complex process with number of challenges. Some of them are very specific for different countries, and it is up to the local researchers to recognize and deal with them. This paper addresses the problem of the infrastructure, i.e. developing of a network of charging stations. Since there are number of specific technical aspects accompanying electric vehicles (types of vehicles, range, charging limitations, price, etc.), the research has started with analysis of the vehicle fleet, road network, and intensity of the traffic in different areas of Republic of Macedonia. This picture is compared with technical characteristics of emerging electric vehicles on the market. That was the way to recognize advantages and disadvantages of use of electric vehicles as substitution of some of the vehicles in the actual fleet. Possible development of use of electric vehicles in the country had to be estimated based on foreign experiences, and such policies in the country. As a result an approach towards development of network of charging stations in Republic of Macedonia has been defined. There is an obvious need this view to be widely presented and discussed with a possible outcome to serve as contribution to the challenges similar countries will face soon.*

Keywords: ELECTRIC VEHICLES, CHARGING STATIONS, TRANSPORT, CHALLENGES

1. Introduction

Electric vehicles are one of the possible innovations capable of helping fighting challenges humanity is facing in the efforts of solving environmental issues.

Being aware that infrastructure is very important part of that process, this paper aims addressing these issues in Republic of Macedonia, especially towards possibilities of development of charging stations network, their types, possible locations, and partially their financing.

Parallel to the technical issues needed to be solved on the electrical vehicles, there is a need of intensive work on development of charging stations network. Since these two aspects are inseparable, development of charging equipment, charging stations, and their network basically depends of the same wide issues mentioning in the context of electrical vehicles. Hence, just as a reminder, common economic environment in which is expected development and use of electrical vehicles, will be mentioned.

Adopting and use of electrical vehicles is considered very limited without stimulation form external factors, like regulations on very limited pollution emission, increasing the fuel price, or financial incentives (Eppstein et al., 2011; Shafei et al., 2012; IEA, 2013). Between these factors, customer incentives have been identified as necessary in order to make use of electric vehicles massive on the market. (Hidrue et al., 2011; Eppstein et al., 2011).

As a consequence of this, the potential of fighting climate changes and use of the electrical vehicles is limited by mentality. Neo-classical economy point that governments policies should be employed to help improvement of such situation. (Rennings, 2000).

On the technical side of the problem, there are number of issues to be solved. Analyses done in this paper represent an effort to recognize the challenges, and make systematic review of the opportunities and limitations in the area of development of electric charging stations in a countries as Republic of Macedonia is.

Dealing in that direction, it is normal to start from the existing structure in the transport sector, i.e. road network, number and type of the vehicles, and intensity of traffic in separate regions of the

country. That will be followed by analysis of the processes of development of electric charging stations in the developed countries, and by presenting of the technical level of the charging stations, themselves. Towards the end, an effort to make comprehensive will be done with aim to identify possible ways of development of charging stations network in Republic of Macedonia. That could lead to identify separate positive and negative aspects of the process.

2. Road transport in Republic of Macedonia

The nature of transport as economy area dictates the need of each country to consider itself as a functional part of regional and global economy. Therefore, smaller countries, first of all, should be aware of global and regional developments, in this case, related to introducing of electrical vehicles in the transport. Understanding of such developments means taking the necessary steps towards avoiding blindness, and recognizing and taking the chances in all possible areas.

As important factors defining the strategy towards introducing vehicles in road transport, several key factors should be considered: road network, registered vehicles, type and intensity of traffic, type of industry, electrical network, legislation and standardization, research and education capacities, etc.

2.1 Road network

Fig. 1 shows road network in Republic of Macedonia. It shows, that besides main international roads, most of the network is concentrated close to the bigger cities/regions.

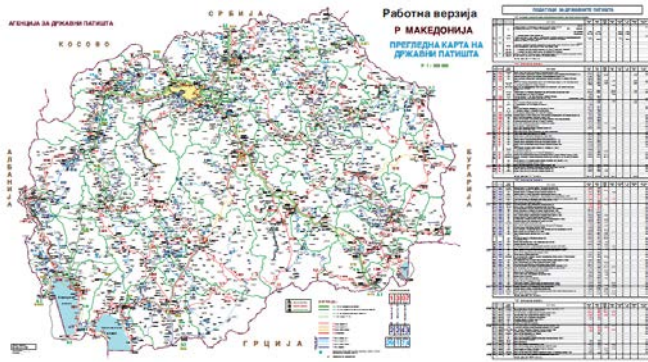


Fig. 1 Road network in Republic of Macedonia

Statistical report of State Statistical Office of Republic of Macedonia [8], gives an overview of road network in the country – tables T-1 and T-2.

T-1: Roads and road categories in km 2012	
TOTAL	14 038
of which asphalt and cobbled roads	8 308
ACCORDING TO ROAD CATEGORY	
Trunk	911
Regional	3 772
Local	9 355
International E-roads	553

T-2: Overview of local roads, situation 31.12.2012 in km		
	Total	Asphalt and cobbled roads
REPUBLIC OF MACEDONIA	9355	4 629
Skopje	551	335
Bitola	167	156
Ohrid	163	97
Shtip	150	39

2.2 Registered vehicles

Table T-3 shows review of registered vehicles in Republic of Macedonia and partially in some of bigger cities [8]

T-3: Registered motor vehicles in 2012			
	Motorcycles	Passenger cars	TOTAL
REPUBLIC OF MACEDONIA	8 473	301 761	350 762
Skopje	3 635	122 400	
Bitola	550	18 961	
Ohrid	573	8 910	
Shtip	237	8 489	

2.3 Road traffic

Main characteristics of road traffic, as one of the key information needed for planning, is shown in table T.4, and T.5, [8]

T-4: Length of E-road according year average daily traffic	
Road length, km	
	2010
Total	550.8
Less than 1000	-
1000 - 1999	13.5

2000 - 3999	195.8
4000 - 5999	194.2
6000 - 9999	41.6
10000 - 14999	105.7
15000 - 19999	-

T-5: Length and use of the roads, 2010						
	Length (km)	Kilometers passed (millions yearly)				
		Total	Motor cycles and three cycles	Passenger cars and light duty vehicles	Load vehicles	Buses
Total length	1724	178.4	2.2	143.5	27.1	5.6
Type of road						
All E-roads	550	63.1	0.1	55.2	6.1	1.7
Total non E-roads	1173	115.3	2.1	88.3	21.0	3.9
Highways	37	0.6	0	0.3	0.2	0.1
Other non E-roads	1136	114.7	2.1	88	2.08	3.8

The number of passengers in urban transport is shown in T.6, [8].

T-6: Number of passengers in towns in thousands, 2012	
Bitola	775
Skopje	68 270
Strumica	224

The table T.7 shows characteristics of Taxi transport [8].

T-7: Taxi transport, 2012	
Passenger cars, number	2 494
Kilometres travelled, in thousands	74 394
Urban and suburban transport	66 911
City to city transport	7 483
Passengers, in thousands	40 413

3. State of the art an expected development of charging stations network in Europe

Figure 2 shows number (in thousands) of charging stations in some European countries in 2012.

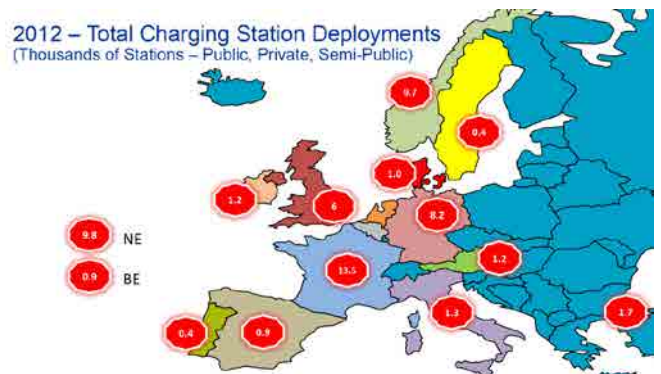


Fig. 2 Number of charging stations in some European countries in 2012 (in thousands)

The number of electric vehicles in the same period presented related to the number of inhabitants (in millions), and the number of public charging stations in Europe is shown on Table T.8.

T.8. Number of electric vehicles related to the number of inhabitants (in millions), and the number of public charging stations in Europe

II. Results in a single overview

The chart answers the knowledge questions and includes the following sections:

Financing indicates who finances the public charging infrastructure in the country:

- Public operator
- Government
- Private

Role grid operator indicates the organisational role of the grid operator:

- Financing
- Connection to distribution network
- Other, such as a role as infra-provider or service provider

Interoperable indicates to what extent there is interoperability between charging stations of different providers:

- Wholly interoperable
- Interoperable between a few providers
- Not interoperable

Switching at station indicates to what extent it is possible to charge using electricity from an electricity company of choice:

- Switching at station is possible
- Switching at station is being investigated
- Switching at station is not possible

Country	Financing	Public grid operator	Interoperable	Switching at station	Number of EV charging stations	Number of EV charging stations per inhabitant	Number of EV charging stations per inhabitant	Number of EV charging stations
1. Austria	H	f	X	X	126	1,047	65	532
2. Belgium	H	f	X	X	73	812	81	895
3. Denmark	H	X	X	X	240	1,398	123	381
4. Estonia	H	f	na	na	106	157	-	-
5. France	H	f	X	X	316	20,000	33	2,100
6. Germany	H	f	X	X	69	7,111	29	2,318
7. Iceland	H	f	X	X	52	254	141	662
8. Italy	H	f	X	X	56	3,315	10	540
9. Netherlands	H	f	X	X	162	9,761	150	3,700
10. Norway	H	f	X	X	2,757	13,626	857	4,029
11. Portugal	H	f	X	X	177	1,852	129	1,362
12. Sweden	H	f	X	X	285	2,368	19	416
13. Turkey	H	f	X	X	8	220	1	52
14. United Kingdom	H	f	X	X	129	8,183	92	3,560

Chapter IV provides an explanation of the information available per country.

Development of the charging stations network is dependable of one industry area which is under development – production of equipment for charging of electric vehicles - EVSE (Electric Vehicle Supply Equipment).

Figure 3 shows the chain containing all key factors in providing electric energy for electric vehicles.

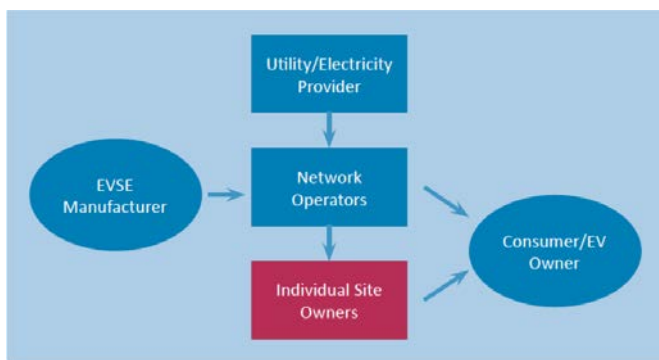


Fig. 3 Chain of supplying electric energy for electric vehicles

Figure 4 shows expected development of charging stations network in EMEA (Europe, Middle East, and Africa) region, i view point of owners, and Figure 5 shows the same view for the key countries in the same region.

Cumulative Public, Private, Semi-Public Charging Station Deployments – EMEA – 000s of Stations

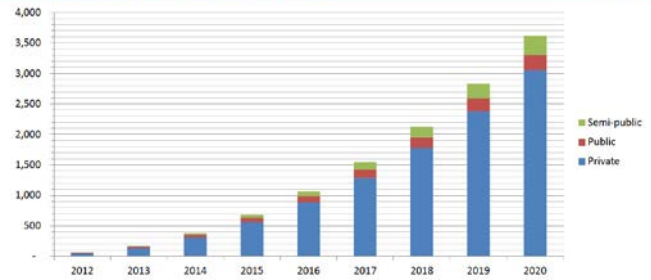


Fig. 4. Expected development of charging stations network in EMEA (Europe, Middle East, and Africa) region

Cumulative Charging Station Deployments – EMEA – 000s of stations

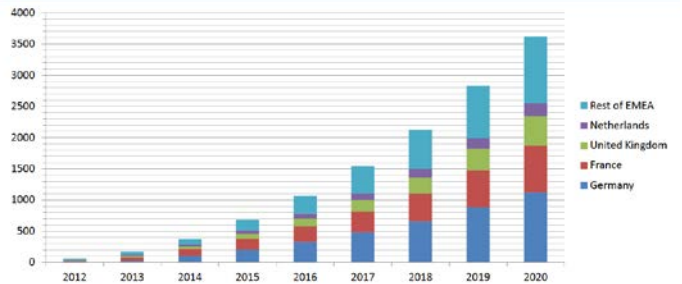


Fig. 5. Expected development of charging stations network in key countries in EMEA

It is widely expected that the number of charging stations in Germany pass the number of one million by 2020, and that number in EMEA region to be higher of 3.6 million.

Besides the number of technical issues which are not closed, like the standardization of charging stations and equipment, all involved, and especially, investors are facing additional business dilemmas. One of the most important is the business model, process forming, etc.

All mentioned makes estimation of profitability difficult, especially for nonresidential charging stations.

The efforts for the estimation start by these factors:

- On the income side:
 - o Existing strategies on forming on the price and business models in which the existing stations are operating at the moment
- On the costs side:
 - o The costs of the equipment and the installations
 - o The price of the electrical energy
 - o Prices of parking
 - o Government subsidies
 - o Price of the capital

Depending of the factors mentioned, the investors use different models in profitability analysis.

Different scenarios are used in the development of network of electric charging stations. Each scenario highly depends of strategies of development of use of electric vehicles. Until massive use of electric vehicles, main elements will be connected with the state policies in the areas of energy, economy and environment. The state support of the businesses in the area of development of charging stations will be very important, as well.

4. Identification of main issues and analysis of possible ways of development of charging stations network in Republic of Macedonia

Analysis of the process of introducing of electrical vehicles, and related to that, development of infrastructure of charging stations is pretty complex process due to lack of mass examples, and even a literature. The research activities and examples are restricted to separate regions, and due to that, different in core elements and content. Therefore it is not possible to come to a clear picture both for the situation and for the predictions. The situation with charging stations is even more complex compared to the electric vehicles, most of all due to the fact it is younger industry.

Based on the undertaken research activities, consultation with experts with years of experience in the area, and described characteristics of the road transport in Republic of Macedonia, several assumptions could be done in relation to the needs and possibilities in the process of introducing of electric vehicles in the country:

- The process of introduction of electric vehicles globally and in Europe is in the first phase of commercialization. In certain vehicle categories, first of all cars, global producers are offering more and more models attractive for different groups of customers.
- There are a number of technical and economic barriers defining that in foreseeable period the use of electric vehicles will be mostly limited to certain categories of vehicles (cars and partially light commercial vehicles), to certain zones (urban, suburban and closed campuses), and to a certain groups of users (municipalities, companies, individuals, etc.).
- Growth of the use of the electric vehicles in most developed economies (US and parts of EU) is expected to be in volume of 20-35% of passenger cars in the next 5-15 years. Use of such vehicles in Republic of Macedonia is expected to be with significantly lower intensity. Also, it is expected that the number of foreign electric vehicles travelling through Republic of Macedonia to be proportionally low. If the starting assumption is that such vehicles would arrive in the country with mostly empty batteries, the plans of building charging stations basically should include zones of crossing the borders, and zones of main crossings of E-roads and E-roads with other main roads. One could expect that the destinations of the foreign electric vehicles entering Republic of Macedonia country would be some of the neighboring countries, the Capital Skopje, some of bigger towns, and main touristic centers, as well.
- The development of the use of electric vehicles in Republic of Macedonia will be directly dependable of the national policy in the energy sector, but also of the policy in the environment protection, as well. The global and Europe experiences show that use of electrical vehicles is related to the urban and suburban areas, especially in the zones with progressive attitude towards environment protection. There a number of reasons that Republic of Macedonia follows such development. That means use of electric vehicles could be most intensive in the areas of the towns Skopje, Bitola, Tetovo, Shtip, Kumanovo, and so on. Maintaining the environmental advantages of the touristic regions is the reason of development of use of electric vehicles in the municipalities of Ohrid, Dojran, Mavrovo, and so on.
- Separate complexes – campuses could have specific attitude towards the environment. The examples could be health centers, education campuses, etc.

- Companies with fleets of passenger cars and small commercial vehicles with urban and suburban operations might be a separate group of users of electric vehicles.
- Taxi companies are one of the main possibilities of using electric vehicles in urban transport.
- Personal use of electric vehicles is very compatible for those families capable of having “second” car for mainly urban and suburban transport.
- There a possibilities of initiatives of production of electric vehicles, and more probably, conversion of the vehicles with engine with internal combustion into electric vehicles.

Main outcomes of the analysis in terms of the challenges and issues to be addressed towards development of the charging stations network in Republic of Macedonia could be grouped in this way:

- In environment of not fully standardized charging equipment, and taking into consideration state of the art and experiences available, and having in mind expected groups of users, there are three levels of ways of charging:
 - o Charging with simple plugs on standard network (220V) (Level 1). This level would be used in home conditions during long (normally by night) breaks of vehicles (mostly personal) use. Such method may be used by some companies having organized parking areas where company fleet of private cars of employees spend significant time.
 - o Charging by special charging equipment with higher power capacity (Laval 2). Their use is appropriate for public parking capacities, big markets, restaurants, and similar places where electric car users spend several hours.
 - o Fast charging stations (Level 3). Charging by this equipment is fast to certain level of batteries capacity and it can be used for additional charging for vehicles whose priority is shortening the time spent at the charging station. This equipment can be used on the main roads, on places like restaurants, existing petrol pumps, motels, hotels, etc. This level could be used as well on public parking, markets, etc. It is very important to have in mind that this type of charging equipment is very expensive and that it is still not clear their possible negative impact on the battery life.

Sustainability of the process of introducing and use of electrical vehicles with its whole complexity (production, conversion, purchase, service, development of charging stations network, etc.) is one of the main issues. All available experiences show that it is so far possible only with strong support and coordination from the government or municipalities. That shows there is a need country to take some of such known forms, or to develop and employ appropriate tools of support.

5. Conclusion

The dynamic nature of this moment of development of electric vehicles and their introduction in service poses significant risk to draw strong conclusions. Accepting it could lead to the following conclusions towards the process of development of network of charging stations in Republic of Macedonia.

It is obvious that the most influential aspect on development of the charging stations network will be the dynamic of introducing of electrical vehicles into service. At the same time, there is a opposite

influence, as well, i.e. charging stations infrastructure has a influence on decisions of buying electric vehicles. It is expected that in visible period of time, use of electric vehicles in Republic of Macedonia will be sporadic, until state takes strong measures in the frames of energy and environment policies.

Electric vehicles will be used, and charging stations network will be developed in urban and suburban areas. Touristic regions and other complexes could be other areas of use.

Government and municipalities fleets could include electric vehicles in some number. Different companies could lead or follow the example.

Electric power in foreseeable period will be used for part of the passenger cars, motorcycles and small commercial vehicles.

Standardisation of the charging equipment is significant precondition to the development of charging stations network.

There is a need of the same nature measures to support the charging stations businesses as those used to support production and market of electric vehicles.

According to the some predictions, the critical point in the development of charging stations network is the transition of dominantly state to dominantly private charging stations. In order to accelerate the process, there is a need of high number of private charging stations.

6. References

[1] UCLA Lewis Center UCLA Institute of Transportation Studies Annual Policy Research Symposium Series Lake Arrowhead The Transportation – Land Use – Environment Connection. Opportunities and Challenges Facing Electric Vehicles David Raney Raney Associates October 17, 2011

[2] Technology, Challenges, and the Future of Electric Drive, MIT Electric Vehicle Team, April 2008

[3] CHALLENGES FOR A EUROPEAN MARKET FOR ELECTRIC VEHICLES, DIRECTORATE GENERAL FOR INTERNAL POLICIES POLICY DEPARTMENT A: ECONOMIC AND SCIENTIFIC POLICY, INDUSTRY, RESEARCH AND ENERGY, **IP/A/ITRE/NT/2010-004 June 2010**

[4] Accenture 2014. The Electric Vehicle Challenge Electric Vehicle Growth in an Evolving Market Dependent on Seven Success Factors

[5] International Economic Development Council, Washington, DC, 2013. Creating the Clean Energy Economy, Analysis of the Electric Vehicle Industry

[6] The Royal Academy of Engineering. ISBN 1-903496-56-X, London 2010. Electric vehicles: charged with potential.

[7] UL, Northbrook, Illinois, 2015. Powering the New Generation of Electric Vehicles: Issues and Challenges

[8] Republic of Macedonia, State Statistical Office, Transport and other services, 2014

PRESERVATION OF POLLUTION OF DANUBE RIVER WATERS

ОПАЗВАНЕ ВОДИТЕ НА РЕКА ДУНАВ ОТ ЗАМЪРСЯВАНЕ

Ass.Professor PhD Kremena Bozhidarova Rayanova
Faculty of Law at "Angel Kanchev" University of Ruse, Ruse, Bulgaria

e-mail: krayanova@uni-ruse.bg

Abstract: *The preservation of ecological system of Black Sea is associated with care for the rivers which flow into it. Bulgaria makes efforts to implement high standards for preservation of the Danube River which represents unique water basin. The improvement of quality of its waters unites the efforts of the riverside countries which contributes for preservation of the ecological system of Black Sea.*

Keywords: POOLLUTION, ECOLOGICAL SYSTEM, DANUBE RIVER, PREVENTIVE MEASURES

1. Introduction

The preservation of ecological system of Black Sea is associated with care for the rivers which flow into it. Bulgaria makes efforts to implement high standards for preservation of the Danube River which represents unique water basin. The improvement of quality of its waters unites the efforts of the riverside countries which contributes for preservation of the ecological system of Black Sea.

The Danube River is unique ecosystem having length of 3000 km¹, on whose river valley live 80 million people. Although the ascertained extinction of many representatives of flora and fauna (arisen of the river pollution and their non-controlled destruction) in the river waters are still found for example 100 species of fish, 300 species of birds and about 400 tree species. In the Danube basin is available very developed agriculture, the river waters are used for irrigation and for production of electricity, it is important transport and communication center, fishing and tourism are developed. Regarding the preservation of the Danube River of pollution the legal regulation of this issue may be specified as relatively recent.

2. Problem discussion.

In the Convention concerning the use of Danube River Waters dating 1958² is available only a general requirement regarding the elaboration and application of measures for avoidance of pollution of the river waters. On 13.12.1985 in Bucharest was approved Declaration of the Danube Countries to Cooperate on Questions Concerning the Water Management of the Danube and in particular by preservation of its waters by pollution³. At it the riverside countries engaged themselves to undertake joint measures by which to avoid and decrease the river pollution. In this regard every country had to ascertain the quality of waters according agreed methods and supervision programs. The results of particular observations, assessments and information were subject to mutual exchange with the purpose of ascertaining and controlling the general condition of Danube. The Declaration affords the establishment of narrow cooperation between the riverside countries, for elaboration of mutual control system and guaranteeing the ecological river safety.

In September 1991 in Sofia city the Danube countries, The Organization for Economic Co-operation and Development, international financial institutions and non-governmental organizations discussed the concept on ecological protection of the Danube River Basin. So was reached the drawing, approval and

opening for signing again in Sofia on 29 June 1994 of Convention on Protection and Sustainable Use of the Danube River⁴. In fact this was the first international legal act by which were regulated the relations between the Danube countries at undertaking measures for preservation of the river waters whose pollution meanwhile has emphasized negative impact also on the condition of Black Sea. In it are provided several basic principles of the modern environmental law, as "pollutant-payer", the right of riverside population to receive current and authentic information about its condition, the implementation of compulsory assessment of the environmental impact of human activities which may have negative impact on the ecosystem.

At the end of 1994 (6-th December) at special international conference of Danube countries, held in Bucharest was approved Declaration for Environmental Preservation in the Danube River Basin. The Ministers of environment of the countries situated on the Danube riverside and the member of the European Union Commission in charge for the environment, territorial planning and civil protection approved at the ecological program for the Danube Basin mentioned above, Danube Strategic Action Plan⁵. It was mainly directed to effective support of the efforts for the soonest possible entry into force of the convention and for the practical application of the convention during the years following its entry into force.

Still in the convention preamble is emphasized the need of cooperation of the Danube countries at the river use and protection which shall be conformed to other international agreements, concerning the condition of the cross-border water streams. On the agreement is also allowed the application of more strict measures at national level with the purpose of improvement of the general condition of Danube waters.

The member-states by the convention have posed two very important aims whose realization is associated with strict ecologically conformable criteria regarding the discharge of waste water in the river and planning different activities which they intend to realize on its riverside. Special attention is drawn to the measures undertaken by Danube countries for limitation, decrease and avoidance of release of substances harming the river waters. In the agreement is emphasized on the preventive nature of measures. They shall be undertaken still at the source i.e. by application of the principle that is better to avoid the pollution than after that to remove its harmful consequences. As key forms of cooperation are determined as the multilateral as well as bilateral consultations, the information, data and experience exchange— mostly when it is about the actions when they shall be undertaken at established or occurred emergency situations. The countries undertook the obligation to implement common emission regulations applicable at the

¹ from Schwarzwald in Germany to its inflow in Black Sea.

² See the text of the Convention in volume 339 of the United Nations Code for international agreements.

³ Although the Declaration is document but not a legal act having mandatory legal force, it still engages at least the political countries to meet the requirements provided in it.

⁴ The Convention was ratified by Bulgarian Parliament on 24.3.1999. It is in force as of 1999 (Revised State Gazette issue).

⁵ See in details the program and plan in Action for a Blue Danube, Arqus-Publishing (Company, Vienna, Austria, 1995)

particular industrial branches and activities. By the texts of the Convention is encouraged the implementation of less-waste and waste-free technologies. For the discharge of waste water in the river was provided the use of permissive procedure. In the drainage Danube Basin shall be made periodical inventories of the point (fixed) and non-point (unfixed) pollution sources. For the purpose shall be drawn lists containing prescriptions for the necessary particular measures. In turn this shall lead to the drawing and application of respective (bilateral or multilateral) action programs. There is also provided the harmonization of monitoring methods as the purpose is to pass to common monitoring system for the whole riverside. In this regard are specified monitoring points and equalized indices on waters quality.

The parties by the convention shall facilitate the submission of best technologies to other countries with the purpose of maximum preservation of the water stream, to establish joint enterprises for environmental friendly productions and to render technical assistance at possibly occurred emergency situations.

Special attention in the agreement is drawn on the establishment and operation of efficient communication warning and alarm systems and plans for emergency reaction and rendering aid to riverside countries suffered by pollution.

For the convention implementation was also established a special international commission whose head office is in Vienna (Austria).

By five appendixes at the convention which are integral part of it were specified some priorities at its application considered for significant.

In the first of them is clarified the issue for use of best available technologies, by encouraging every initiative which may lead to their further development and elaboration. At application of these technologies is significant to be outlined their preventive role, they shall be used in a manner which contributes for avoidance of ecological risk and also by them shall be assisted passing to activities which are less polluting the environment.

In the second appendix are included the industrial branches and hazardous substances, on which the member states shall pay special attention. In fact it is about the activities which are most risky for the environment as power engineering, ore output and metallurgy. The operation of such branches often leads to the release of substances which are hazardous for the river waters: radioactive, mercury, cadmium, heavy metals etc.

The third one refers to the purposes, which the countries pose and the criteria, which shall be applied for improvement of waters quality. The idea is the same to be maintained at condition which is environmentally friendly. Hence is the undertaking of the countries by the agreement to decrease the discharge in the river of waste water and in particular hazardous substances. If necessary there maybe posed specific requirements regarding some water categories as well as in particular river areas which are more delicate in ecological manner.

In the fourth appendix is specified the statute of the International Commission for preservation of Danube River established by virtue of the convention itself: members of the commission – functions, powers, capacities etc., chairmanship, summoning conferences of the member-states, manner of approval of decisions and recommendations. The Commission is entitled to establish permanent working groups on specific problems and activities regarding the preservation and sustainable use of Danube River. There was also established a special secretariat having head office in Vienna whose main task is the collection and distribution between the member-states of information regarding the convention, assistance of the operation of the international commission, implementation of technical and legal services and consultations etc.

3. Conclusion.

Regarding disputes solving by interpretation and application of the convention in special (fifth) appendix was provided arbitral procedure. For the purpose is established Arbitral Court which takes its decisions according the regulations of international law and the ones included in the convention itself.

4. LITERATURE

[1]. Convention in volume 339 of the United Nations Code for international agreements

[2]. Program and plan in Action for a Blue Danube, Arqus-Publishing (Company,Vienna,Austria,1995)

[3]. Belgium, Great Britain, Denmark, Norway, France, Federal Republic of Germany, the Netherlands and Sweden

[4]. Tomov, V. Risk theory. Monography, Ruse, University of Ruse, 2003, page 440

[5]. Tomov, V. Diagnostics of environmental safety. Dissertation for obtaining academic degree “Doctor of Economic Science”. Ruse, University of Ruse, 2006, page 445

[6]. Cf. Manuel sur la pollution par les hydrocarbures,, OMCI, Londres, 1972.

INTERNATIONAL LEGAL MEASURES FOR AVOIDANCE OF SEA POLLUTION WITH PETROL

МЕЖДУНАРОДНОПРАВНИ МЕРКИ ЗА ПРЕДОТВРАТЯВАНЕ НА ЗАМЪРСЯВАНЕТО НА МОРЕТО С НЕФТ

Chief Asst. PhD Vanya Velichkova Panteleva
Faculty of Law at "Angel Kanchev" University of Ruse, Ruse, Bulgaria

e-mail: vpanteleva@uni-ruse.bg

Abstract: *The problem for pollution of sea environment is universal and has diverse aspects and indications. At its solving is worked in two directions. On the one hand - by establishment and elaboration of the technical methods and on other hand-by preparation, coordination and approval of legal acts.*

Keywords: LEGAL MEASURES, AVOIDANCE, SEA POLLUTION, PREVENTIVE MEASURES,

1. Introduction

The problem for pollution of sea environment is universal and has diverse aspects and indications. At its solving is worked in two directions. On the one hand - by establishment and elaboration of the technical methods and on other hand-by preparation, coordination and approval of legal acts.

The different countries are interested in different degree of the fight against pollution depending on their natural and economic resources. At them belong: access to the sea coast, demographic density of this coast, level of economic development, need of petrol. The measures taken individually by the countries do not guarantee safety. It is possible unilaterally taken measures not to be approved or respected. Less or generally not interested countries may not respect regulations stipulated by international agreement.

2. Problem discussion.

Therefore one of the special features in this field is expressed in diversity of interests and the arising difficulty for finding balance between them.

1. Technical methods

The countries as well as the specialized international organizations and institutions investigate and apply particular technical methods, aim to implement new technologies with the purpose to eliminate or at least to minimize the pollution risks. It is appropriate for their assessment to be made according the method of integral risk^{1 2 3}

The used traditional technical methods for fight against the petrol fallen into the marine environment occurred ineffective from ecological point of view. The petrol cover processed by chemical means may visibly disappear. However the solvents used for neutralization of the pollution source are very often more hazardous for the sea flora and fauna than the petrol itself⁴.

The coagulants (chalk, different types of shavings etc.) do not remove the petrol spilled on the water surface. At the same time its burning is practically impossible as it is ignited very hard.

The method of pumping the petrol at the sea surface is applied by absorption and pouring in the cisterns of tankers or in light

rubber tanks. But this method is not sufficiently efficient due to the limited flow rate of the pumps. There are also used specially constructed ships equipped with absorption devices which pump the spilled petrol.

However the practice shows that the use of technical methods may not solve the problem for the sea pollution completely. Moreover there is not yet developed and implemented satisfactory method for efficient cleaning of polluted sea waters. Even the most perfect devices in particular cases may not be used rationally and with their full capacity due to concrete atmospheric conditions, specific sea flows, wind force and direction, condition of the spilled petrol etc⁵. In addition the simple and harmless mechanical cleaning is difficultly applicable at very large water areas polluted with petrol.

The use of technical means for fight against pollution of sea environment with petrol does not belittle the legal aspect of the PROBLEM, because the activity of countries by sea is regulated by the norms of international law. The chemical, mechanical and other applied methods for fight against pollution may and shall be used mainly at incidental petrol spillages, i.e. at absolute necessity-after all conscientiously taken precautions for avoidance of pollution have already been undertaken.

2. Legal methods

The preparation, coordination and approval of legal norms for protection and preservation of the sea of pollution also meets many difficulties⁶. It may be noticed that until recent times the international law showed great restraint regarding pollution. The laconism in this field is explained with the different statements on this issue some of which are due as L. Kavare notes "to the lack of international solidarity and of the resistance showed by the countries".

In order to be more precisely and more correctly estimated the attempts undertaken for solving the sea pollution problem, it shall be noted that it has double aspect. It may be concerned on one side for pollution of the country coasts and for recovery of the caused damages. On other side it may concern for pollution of the deep sea which is declared for "common possession of the humanity". But unfortunately still nobody may claim recovery of damages caused by the deep sea pollution. There are no provided and maybe is difficult to be provided the rules for damages recovery, caused by the pollution of the deep sea.

The intentional spillage of petrol and petrol waste became frequent occurrence. It led to undertaking conventional measures in

⁵ Belgium, Great Britain, Denmark, Norway, France, Federal Republic of Germany, the Netherlands and Sweden

⁶ Tomov, V. Risk theory. Monography, Ruse, University of Ruse, 2003, page 440

¹ Held in the period 24.02-27.04.1958

² See Al. Yankov, Towards new international legal regulation..., page 40

³ Art. 24 of the Convention on the Deep Sea

⁴ See. L. V. Speranskaya, Международно-правовая охрана морской среды, М., 1978, с. 80-81; Материалы по морскому праву и международному торговому мореплаванию, вып. 11/1976, page. 38-39.

international aspect with the purpose to avoid the devastating effects of the marine environment pollution. First positive result in this regard was achieved by the approval of the Convention dating 1954.

The Geneva Convention on the Law of the Sea⁷ (important from the point of view of the attempt for codification of its principles) in fact has not brought anything new on the issue for avoidance of pollution of the marine environment⁸. It shall be noted that at this Conference was not determined the definition of this occurrence, its action and indication mechanisms in the time and space. The Conference also has not provided what shall be the measures which the countries may undertake for fight against pollution. As for the issue about water areas in which the countries may interfere for pollution avoidance the conventions approved at the Conference also kept silence. So art. 24 of the Convention on the Territorial Sea and the Contiguous Zone as well as art. 6 of the Convention on Fishing and Conservation of the Living Resources of the Deep Sea represent only principle declarations containing general provisions.

As a result of more frequent incidental petrol spillages (very indicative in this regard was the case with "Torrey Canyon" in March 1967 which became reason for serious drawing of the attention of the global publicity on the arisen legal problems at such spillages), occurred the necessity for entitlement of the countries to interfere in the deep sea in the cases of incident leading to petrol pollution. This was expressed in concrete form by approval of the Convention on the Right of Interference.

In the rules included in Appendix I at the MARPOL 73 Convention the greatest attention is drawn to the requirements regarding ships (and especially the tankers) for removal of the reasons for petrol pollution at the different types of sea operations, related to their normal operation.

3. Preventive measures undertaken at national level

The undertaking of such measures is of the jurisdiction of the countries taken individually. The general rules are that "every country undertakes to issue Ordinances for avoidance of sea pollution with petrol of ships..."⁹. Within their jurisdiction the countries provide respective measures for avoidance of sea pollution. These measures are related to the activity exercised by the country within its jurisdiction. The coastal country has as the right as well as the obligation to avoid the pollution of its territorial sea. It is bridge between the deep sea and the territory. That is why the coastal country shall require observance of its cleanliness as on behalf of its citizens as well as on behalf of the citizens of foreign countries.

However when it is about the waters of the deep sea which due to its specific nature may change its location for some reason, the internal legislation may not provide specific measures against their pollution and even less to prevent it as it may occur in indefinite part of the sea areas. Moreover, according internal legal order is practically difficult to be established efficient system for control over pollution and to be determined the range of its statute. The individual and isolated initiative may not preserve the interests of the country at pollution, no matter what is the preciseness of the undertaken legal measures. This is due to the fact that the modern international law even acknowledging sovereign prerogatives of the countries, is limiting their place of effect. Also due to the actual unity of the sea waters any of the countries may delimitate a particular coastline completely protected by pollution risks. On the

other hand the status of deep sea is not regulated by national laws but of international regulations which until recently in considerable degree were limiting the jurisdictions of the particular countries. At this the deep sea remains zone in which the pollution risks are significant.

Individual, isolated initiative shall be undertaken only at absence of international regulation or in the cases of incompleteness of the last. In any case is necessary the same to be conformed to the common obligation of the countries to undertake the respective measures for avoidance of the sea environment pollution.

4. Preventive measures undertaken at regional level

The United Nations Organization, its specialized organizations and authorities are not the only one which deal with the issues on sea pollution. Between the countries was established cooperation and in more limited frameworks (regional or affecting particular geographic surface, favorable for the undertaking of collective preventive measures). It had proven to be very effective because it is realized between countries which are directly interested in the fight against sea pollution, on whose coasts they are located.

Another agreement at regional level was the signed 22.03.1974 in Helsinki between the seven Baltic countries¹⁰ Convention on Protection of Sea Environment in Baltic Sea Area. In the provisions of the Convention as well as in the appendixes at it are comprised different types of marine environment pollution (including also at research and exploitation of the sea bottom and its bowels-art. 10) and the fight against them. The contracting countries undertake to take the necessary measures for avoidance and removal of pollution. (art. 3, p.1). They shall cooperate at the investigation of breaches of conventional prescriptions for pollution avoidance – check of the boarding documents, sample taking etc. An important part of the regulations included in the Convention is dedicated to the problem of pollution of sea waters by ships (art. 7 and the measures provided in Appendix IV). After the example of MARPOL 73 Convention, in these rules is also made delimitation between the different cargo components, waste water and sediments. Each Baltic country undertakes the obligation to equip its ports and terminals with the respective reception devices for waste of the ships visiting them (petrol sediments, hazardous substances etc.)- art. 7. The Parties by the Convention undertake the obligation to render assistance to IMCO at preparation of navigation rules for the straits and shallows of Baltic Sea, in order to avoid the cases of incidents.

There is no doubt that the Helsinki Convention is very complete and comprises all aspects of the fight for avoidance, decrease and removal of pollution. It provides sufficient guarantees for preservation and improvement of the sea environment in the region of Baltic Sea.¹¹

In the beginning of 1976 in Barcelona was held Conference of the countries of Mediterranean Basin¹². On it was approved Convention on Avoidance and Limitation of Pollution of the Mediterranean. In its provisions is provided as the undertaking of measures against pollution caused by human activity by sea – by ships, aircrafts, research and operation of continental shelf as well as of any type of ground sources (art. 6-8). To the parties is imposed the obligation to undertake all necessary individual or joint measures for avoidance, limitation and fight against pollution of the Mediterranean. (art. 4). Unlike the Helsinki Convention this one does not provide rules additional to MARPOL 73. For it is satisfactory to declare that the contracting parties undertake to take

⁷Tomov, V. Diagnostics of environmental safety. Dissertation for obtaining academic degree "Doctor of Economic Science". Ruse, University of Ruse, 2006, page 445

⁸ Art. 1 of the Agreement

⁹German Democratic Republic, Denmark, Poland, USSR, Federal Republic of Germany, Finland and Sweden

¹⁰ See in details Л.В. Сперанская, quote. съч., page 63-8-. The text of the Convention in Материалы по морскому праву и..., вып. 21/80, page. 83 and the following.

¹¹Excluding Albania and Algeria. The Convention was signed on 16.02.1976

¹² Art. 2 of Geneva Convention of 1958 for deep sea

all measures provided by the international law for fight against pollution of the Mediterranean, caused by ship spillages.

The examples listed above for regional cooperation in the fight against marine environment pollution may be qualified as successful and appropriate forms for mutual cooperation within the global efforts for limitation and removal of the pollution hazard.

5. Preventive measures undertaken at global level

The international nature of the sea environment pollution problem is conditioned by the following circumstances:

- the reason for the possible damages of pollution may be accident in deep sea where the freedom of navigation is acknowledged to all countries¹³. And the navigation is international as regarding the ship flag as well as regarding its destination;

- interest of all countries in pollution avoidance notwithstanding if they are coastal or not. The pollution may concern any part of the Global Ocean and all countries have attitude to this problem, because in most of the cases of pollution are concerned in one or another degree the interest of the whole international community. The protection and preservation of the deep sea resources which belong to all countries including the ones without coast are of crucial importance. As source of resources the sea is beyond the control of the individual country. As source of resources it may be used efficiently on the way of international cooperation. Or as it is mentioned in art. 25, p. 2 of the Convention on Deep Sea, "all countries undertake to cooperate with the competent international organizations at taking measures for avoidance of sea pollution ...".

Every country is entitled to take individual measures within its jurisdiction but such measures may not lead to complete solution of problem having international legal nature. It is true that the exercising of this right may be of favor not only for this country because at undertaking measures in its own interest against occurred pollution hazard at the same time it acts in interest of the international community– the undertaken measures contribute for preservation of the sea environment cleanliness. Nevertheless there are no guarantees that the individual preventive measures shall be favorable for any other particularly interested country. They may have negative consequences also for third countries or for the common interests of humanity. That is why it would be impossible the initiative for these measures to be left entirely to the countries taken individually without exercising any control on them. Such control may be organized only within international conventions. As example in this regard may be indicated the Convention on the Right of Interference. The countries which are parties on it are entitled to undertake in deep sea the necessary measures for avoidance of the sea environment pollution (art. 1 of the Convention). At the same time they undertake to observe the limitations arising of art. 5 of the same convention and namely – proportionality between measures and damages, termination of measures by realization of purpose, criteria at estimation of measures.

However at all cases until the entry or entering into force of a particular convention the national legislations have key role for the application of the regulations provided in the convention concepts. It is realized by means of the preparation of respective internal legal norms.

3. Conclusion.

There is no doubt and is in common interest the international law to provide by its own means the protection and preservation of the sea by petrol pollution. By its nature the international legal regulations in this area have more expressed preventive nature and the institute of the liability provided by it has wider perimeter of the one of the established and applicable rules of responsibility for the

damages caused at sea transport. However the responsibility at pollution may find particular application by establishment of proper and specific procedures. Their task is to provide the observance and application of the formulated rules as well as their adaptation to all circumstances which may change very fast. It is typical that all entered conventions concerning the problems with petrol pollution of the sea aim to respond to this requirement.

LITERATURE

- [1]. Held in the period 24.02-27.04.1958
- [2]. See Al. Yankov, Towards new international legal regulation..., page 40
- [3]. Art. 24 of the Convention on the Deep Sea
- [4]. See. L.V. Speranskaya, Международно-правовая охрана морской среды, М., 1978, с. 80-81; Материалы по морскому праву и международному торговому мореплаванию, вып. 11/1976, page. 38-39.
- [5]. Belgium, Great Britain, Denmark, Norway, France, Federal Republic of Germany, the Netherlands and Sweden
- [6]. Tomov, V. Risk theory. Monography, Ruse, University of Ruse, 2003, page 440
- [7]. Tomov, V. Diagnostics of environmental safety. Dissertation for obtaining academic degree "Doctor of Economic Science". Ruse, University of Ruse, 2006, page 445
- [8]. Art. 1 of the Agreement
- [9]. German Democratic Republic, Denmark, Poland, USSR, Federal Republic of Germany, Finland and Sweden
- [10]. See in details Л.В. Сперанская, quote. съч., page 63-8-. The text of the Convention in Материалы по морскому праву и..., вып. 21/80, page. 83 and the following.
- [11]. Excluding Albania and Algeria. The Convention was signed on 16.02.1976
- [12]. art. 2 of Geneva Convention of 1958 for deep sea
- [13]. Tomov, V, Risk theory. Monography, Ruse, University of Ruse, 2003, page 440
- [14]. Cf. Manuel sur la pollution par les hydrocarbures,, OMCI, Londres, 1972, p. 13
- [15]. L. Caavaare, op.cit.p ., 617

¹³ Tomov, V, Risk theory. Monography, Ruse, University of Ruse, 2003, page 440

IDEOMOTORIC TRAINING AS A TOOL FOR PROFESSIONAL RELIABILITY IMPROVEMENT AMONG POLICE OFFICERS

ИДЕОМОТОРНАЯ ТРЕНИРОВКА КАК СРЕДСТВО ПОВЫШЕНИЯ ПРОФЕССИОНАЛЬНОЙ НАДЕЖНОСТИ ПОЛИЦЕЙСКИХ

As. prof., dr. psych. Kalinnikova, L.¹, ma. psych. Zavodilov, A.²
Baltic International Academy¹, "Psy Technology" LLC^{1,2} - Latvia
e-mail¹ : kalin.l@inbox.lv; e-mail² : aleksejs_zavodilovs@inbox.lv

Abstract. Professional activity of police officers is often related to extreme situations stimulating the emergence and development of stress conditions. Police officers, who were not trained in dealing with stress, in extreme situations, can act in a professionally inappropriate manner and put at risk (including risk of death) those involved in a situation, including police officers themselves, and deteriorate the efficiency of resolving the situation of offence. Lack of skills on how to cope with stress significantly undermines normal activity of police officers. The article discusses the theoretical basis of the authors' developed ideomotoric training program designed for police officers, as well as its validation results. The program aims to decrease the negative consequences of being emotionally involved in stressful situations and to enhance the individual resistance to stress among police officers. The special attention is focused on professional reliability improvement among police officers resulting from participation in the ideomotoric training program.

KEYWORDS: IDEOMOTORIC TRAINING, MENTAL IMAGE, SELF REGULATION, STRESS, STRESS FACTORS, EMOTIONAL REACTION TO STRESS.

1. Introduction

Ensuring collective security is the primary task of police officers, especially taking into account the changing conditions in Europe. The number of situations that, potentially, can be dangerous in terms of provocative actions leading to aggravation of the situation in the region and the confrontation of parties has been increasing. Accordingly, increased the number of emergency situations with the involvement of police officers. Current scientific views indicate [1,2] stress as the main component of extreme police activity. Increased levels of stress accompanied with lack of coping skills endanger normal life of police officers, lead to professional errors and discipline violations, decrease the sense of responsibility, reduce the quality of family life [3], result in negative health conditions [4, 5], can lead to sleep deprivation, alcohol abuse, psychological discomfort (anxiety, frustration, depression), community complaints and dismissals from work [5]. Many of abovementioned facts can be explained by the development of emotional disturbances leading to destructive changes in the personality of a police officer (professional deformation) and efficiency of his/her labour. Among police officers, the following negative emotional responses to stress has been revealed: anger, agitation, recklessness, anxiety, frustration, uncertainty [7]. When blocking an urge to act in a stressful situation, aggressive impulses can result in an unacceptable harmful behaviour towards other people (disciplinary violations and breach of orders) or be projected onto people who are not involved in the situation (colleagues, friends, family members). Frustration and lack of confidence can lead to the *learned helplessness* development, a condition which is characterized by apathy, detachment and inaction in response to events beyond the control of an individual [6]. Anxiety (constant inner restlessness) can be manifested in reduced concentration abilities, anticipation of negative consequences, uneasiness, irritability, restlessness, increased fatigue levels, which leads to erroneous actions, alcoholism.

Therefore, improving psychological resistance to stress in police officers is professionally important because it is directly related to security safeguarding.

For this task, the method of ideomotoric training was chosen among the scope of methods used for learning self-regulation of negative psycho-emotional conditions. The benefits of this method are short implementation period, internal resource management, increased stress resistance, regulation of emotional state, and elimination of negative thoughts.

According to previous research, in an ideomotoric act mind and body are jointly engaged. The physiological mechanism of ideomotoric reactions was first explained by Pavlov, who highlighted the role of language and visual images forming the act. Later, Luriya described the mechanism of conditioned reflex reactions that lead to the desired result by means of re-playing a mental image, while performing conscious muscle relaxation. As a result of this training, in extreme/nonstandard situations motor movements provoke automatic response on the unconscious level. The basis of this approach is a mental repetition of own actions in different situations, thus, it can be suitable in police training. Modern theory of bioinformatics (Taylor, 1995) focuses on a mental image creation as a self-regulation skill. The self-regulation process involves two components: pre-programming activities and program manifestation in behaviour. Therefore, the mechanisms of an ideomotoric act can be implemented for improving psychological regulation skills. According to Sandomirsky [8], the main conditions for an ideomotoric act are a mental image creation and a minor relaxation. To comply with these conditions in the self-regulation training program for police officers, a reverse mechanism of ideomotoric reactions was implemented, i.e. the execution or simulation of certain simple movements promote generation of individual images and exempt from intrusive thoughts or negative emotions. The exercises implemented in the program consisted of short simple actions performed simultaneously in an individual rhythm. Ideomotoric movements performed in such a mode result in relaxation, which enables activation of mental images and set ups. Before the start of the training, each participant reported which would be the desired state or feeling when exposed to an extreme situation. It was required in order to create an accurate image of the desired psychophysiological state. As a result, in a stressful situation, the activation of a dominant mental image leads to desired physiological conditions and emotional reactions on the automaticity level. The following patterns of the ideomotoric training were taken into account during the training program implementation: participants' motivation and systematic and distinct sequence of the exercises. When analysing the results of the ideomotoric training its delayed effect was considered as a pattern: for each individual the effect of the training can be manifested after different time periods.

2. Method

The current research is a pilot study aiming to analyse the efficiency of the ideomotoric training method.

The main hypothesis: there is a difference in the modality of emotional responses to stress in a group of police officers who underwent the ideomotoric training and those who did not participate in the training.

Participants: Thirty police officers employed by the State Police, all men. Participation was voluntary. Sample type – a convenience sample. Participants were divided into two groups: experimental (ideomotoric training, N=15), and control (N=15). Participants' mean age in the experimental group M= 34.5, in control group M=34.4.

Measures: Emotional Stress Reaction Questionnaire (ESRQ) developed by Larsson [9].

Training instrument: Ideomotoric training program.

Procedure: The study was run from January to March 2016. Before the ideomotoric training, a pre-test (ESRQ) was administered in both groups to evaluate the dominant emotional reaction to stress - positive or negative. The test was used retrospectively. Previously, it was revealed that contacts with people in a state of panic and contacts with aggressive-minded people are the situations treated by the police officers as the most extreme and stressful, potentially leading to losses, very dangerous and demanding large energy inputs. The most often mentioned situation, a contact with aggressive-minded people, was selected to assess the emotional response to stress. After the evaluation, participants assigned to the experimental group participated in a 10-session ideomotoric training. Total training time - 150 minutes (2 hours and 30 min). After the ideomotoric training, a post-test was administered to both groups (ESRQ) to evaluate the dominant emotional reaction to stress after the ideomotoric training in the experimental group and without training in the control group.

3. Results and Discussion

The analysis of the pre-test results obtained with the ESRA questionnaire revealed heterogeneity of the emotional response to stress in the experimental and control groups (Fig.1). In both groups, the reaction to stress was negative, however, in the experimental group the performance was slightly worse. The range of indicators in the post-test condition was substantial in both groups. The post-test revealed that after the ideomotoric training in the experimental group the reaction to stress improved and became positive, whereas, in the control group the indices did not change demonstrating that emotional reaction to stress remained at the same negative level.

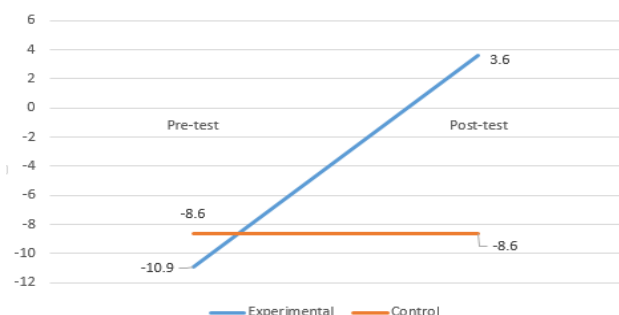


Fig.1. Pre-test and post-test indices in both groups

Fig.1 demonstrates the heterogeneity of the experimental and control groups. This is due to the small pilot sample and certain characteristics of the real group. Since the assumption of homogeneity of regression slopes is broken, the ANCOVA analysis can not be implemented for the results analysis. Therefore, to identify the differences between the two groups before and after the ideomotoric training the Mann-Whitney U-test was implemented. This test also allows to detect differences in small samples.

Table 1 shows mean ranks in experimental and control groups before and after the ideomotoric training.

Table 1. Ranks

	Group	N	Mean Rank	Sum of Ranks
Before Training	Experimental	15	12.17	182.50
	Control	15	18.83	282.50
After Training	Experimental	15	23.00	345.00
	Control	15	8.00	120.00

Table 2 demonstrates the U-criterion values and probabilities.

Table 2. Test Statistics

	Before Training	After Training
Mann-Whitney U	62.500	.000
Wilcoxon W	182.500	120.000
Z	-2.090	-4.678
Asymp. Sig. (2-tailed)	.037	.000

The data analysis revealed that there were statistically significant differences in emotional responses to stress in the experimental and control groups. Before the ideomotoric training, the negative stress response was more pronounced in the experimental group ($Mdn = -10$), than in the control group ($Mdn = -9$), $U = 62.5$, $p = .034$. However, after the ideomotoric training conducted in the experimental group, the emotional response to stress in this group become positive ($Mdn = 4$), in contrast to the control group ($Mdn = -9$), $U = 0$, $p < .001$.

According to Larsson [9], positive emotional reaction to stress indicated by the scale points out that the subject perceives one's condition after a stressful situation as an active. Thus, police officers see themselves in a state of alert, indicating tranquillity, activity, concentration and focus. Negative responses to stress are associated with a sense of threat, indifference, sense of uncertainty and anxiety, anger, uncontrolled aggression. The results of the study revealed the effectiveness of ideomotoric training in the experimental group, despite the short duration of its implementation.

4. Conclusions

The results of this study allow to draw the following conclusions:

- The main operation hypothesis, that there is a difference in the modality of emotional responses to stress in a group of police officers who underwent the ideomotoric training and those who did not participate in the training, has been confirmed.
- Statistically significant differences in emotional responses to stress in the experimental and control groups revealed.
- The obtained results indicate the effectiveness of the ideomotoric training, despite screening conditions.
- The ideomotoric training allows to change the psycho-physiological and emotional state of police officers exposed to stressful situations.

5. References

- [1]. Bond, M. (2014). The Impact of Stress and Fatigue of Law Enforcement Officers and Steps to Control It. - American Military University. February, 24.
- [2]. Collins, P., Gibbs, A. (2003). Stress in police officers: a study of the origins, prevalence and severity of stress-related symptoms within a country police force. In: Occupational Medicine. Vol. 53, Nr.4.
- [3]. Balinska, B. & Wiciak, I. (2012). Fatigue and professional burnout in police officers and firefighters. In: International Security, 4 (2). – 265-273 p.p.

- [4]. Senja, S. (2011). Dangerous fatigue conditions: A study of police work and law enforcement administration. In: *Police Research*, 12 (3). – 235-252 p.p.
- [5]. McCarty, W., Schuck, A., Scogan, W., Rosenbaum, D. (2011). *Stress, Burnout and Health. - Topical Report. National Institute of Justice. January, 2011.*
- [6]. Wortman, C. & Brehm, J. (1975). Response to uncontrollable outcomes: An interpretation of reactance theory and the learned helplessness model. In: *Advances in experimental soc. psychology*. L. Berkowitz (ed.). Vol.8. - N.Y.: Academic Press.
- [7]. Charoen, P. (1999). *Officer involved shooting: the emotional impact and effective coping strategies. – University of Nevada. – Las Vegas. December, 1999.*
- [8]. Сандомирский, М. (2007). *Психосоматика и телесная психотерапия. – М.: Класс. – 592 с.*
- [9]. Larsson, G. (2011). *The Emotional Stress Reaction Questionnaire (ESRO): Measurement of Stress Reaction Level in Field Conditions in 60 Seconds. – Karlstad. Swedish National Defence College*