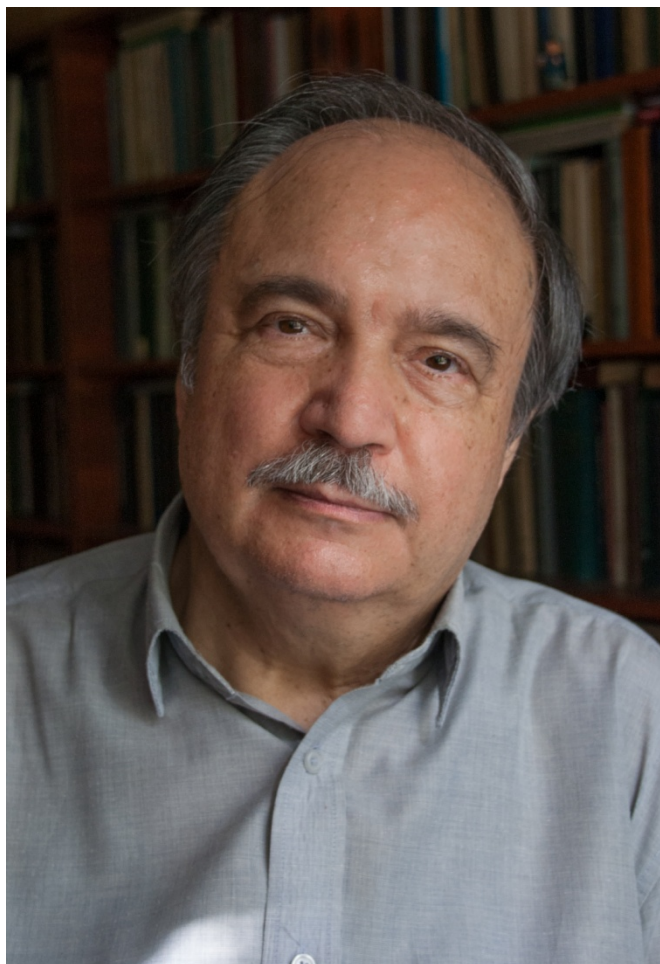


INTERNATIONAL SCIENTIFIC JOURNAL

MATHEMATICAL MODELING

YEAR I, ISSUE 4/2017
ISSN (PRINT) 2535-0986
ISSN (WEB) 2603-2929

Published by
SCIENTIFIC-TECHNICAL UNION of MECHANICAL ENGINEERING - INDUSTRY 4.0
Sofia, BULGARIA



Уважаемые коллеги!

Задача нашего журнала – предоставить возможность широкой научной общественности познакомиться с новыми идеями и исследованиями теоретического и прикладного характера из разных областей научного творчества, но объединенных общим языком описания – языком математики. Использование этого языка позволяет лучше осознать единство и взаимозависимость различных, на первый взгляд, явлений и процессов. Мы надеемся, что наш журнал поможет молодым исследователям научиться грамотно излагать свои мысли, а также сможет подсказать им новые направления для творческого поиска. Мы надеемся также, что журнал сможет стать ареной содержательных профессиональных дискуссий, ибо, как хорошо известно, «в споре рождается истина». Со своей

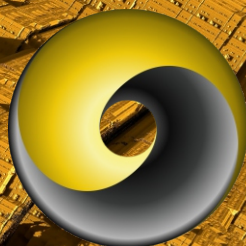
стороны, мы сделаем все от нас зависящее, чтобы создать для авторов комфортные и объективные условия общения с Редакционной коллегией. Успехов!

Dear colleagues!

Our journal is aimed to provide an opportunity for the wide-range scientific community to get acquainted with new ideas in theoretic and applied research, in various areas of scientific creativity, united by a common language - the language of mathematics. This language is able to clarify an understanding of the unity and interdependence of phenomena and processes, which initially are seemed to be different. We hope that our journal could be helpful for young researchers, who want to learn how to express correctly their thoughts, and also show them new directions of creativity. We hope that our journal will become an arena for meaningful professional discussions, cause, as it's well known, "Discussio mater veritas est". For our part, we will do our utmost to create comfortable and objective conditions for communication of authors with the Editorial Board. Good luck!

Andrei Firsov

INTERNATIONAL SCIENTIFIC CONFERENCE



MATHEMATICAL MODELING PROCESSES AND SYSTEMS

13-16. DECEMBER 2017, BOROVETS, BULGARIA

ORGANIZERS

SCIENTIFIC-TECHNICAL UNION of MECHANICAL ENGINEERING - INDUSTRY 4.0
BULGARIA

PETER THE GREAT ST.PETERSBURG POLYTECHNIC UNIVERSITY
RUSSIA

BULGARIA, Sofia 1000, 108 G.S.Rakovski Str., office 411
phone: + 359 2 987 7290

office@mathmodel.eu <http://www.mathmodel.eu>

INTERNATIONAL EDITORIAL BOARD

EDITOR I CHIEF

Prof. ANDREY FIRSOV Peter the Great St.Petersburg Polytechnic University	RU
---	----

Members:		
Abilmazhin Adamov, Prof.	L.N.Gumilyov Eurasian National University	KZ
Alexander Guts, Prof.	Omsk State University	RU
Alexei Zhabko, Prof.	Saint Petersburg State University	RU
Andrey Markov, Prof.	Baltic State Technical University	RU
Andrii Matviichuk, Prof.	Kyiv National Economics University	UA
Andrzej Nowakowski, Prof.	University of Lodz	PL
Anton Makarov, Dr.	Saint Petersburg State University	RU
Armands Gricans, Assoc. Prof.	Daugavpils University	LV
Artūras Dubickas, Prof.	Vilnius University	LT
Avinir Makarov, Prof.	Saint Petersburg State University of Industrial Technologies and Design	RU
Christo Boyadjiev, Prof.	Institute of Chemical Engineering, BAS	BG
Daniela Marinova, Dsoc. Prof.	Technical University of Sofia	BG
Dimitrios Poulakis, Prof.	Aristotle University of Thessaloniki	GR
Evgeniy Smirnov, Assoc. Prof.	Volgograd State Technical University	RU
Giovanni Borgioli, Assoc. Prof.	University of Florence	IT
Haskiz Coskun, Prof.	Karadeniz Technical University of Trabzon	TR
Idilia Bachkova, Prof.	University of Chemical Technology and Metallurgy	BG
Igor Anufriev, Assoc. Prof.	Peter the Great St.Petersburg Polytechnic University	RU
Irena Stojkovska, Prof.	Ss. Cyril and Methodius University in Skopje	MK
Ivana Štajner-Papuga, Prof.	University of Novi Sad	RS
Kanagat Aldazharov, Assoc. Prof.	Kazakh Economics University	KZ
Karl Kunisch, Prof.	University of Graz	AT
Mahomed Agamirza ogly Dunyamalyev, Prof.	Azerbaijan Technical University	AZ
Marius Giuclea, Prof.	The Bucharest University of Economics Studies	RO
Mihail Okrepilov, Prof.	D.I. Mendeleev Institute for Metrology (VNIIM)	RU
Milena Racheva, Assoc. Prof.	Technical University of Gabrovo	BG
Mohamed Kara, Dr.	Ferhat Abbas Sétif 1 University	DZ
Mohamed Taher El-mayah, Prof	MTI University	EG
Neli Dimitrova, Prof.	Institute of Mathematics and Informatics, BAS	BG
Nina Bijedic, Prof.	Dzemal Bijedic University of Mostar	BA
Oleg Obradović, Prof.	University of Montenegro	ME
Olga Pritomanova, Assoc. Prof.	Oles Honchar Dnipropetrovsk National University	UA
Özkan Öcalan, Prof.	Akdeniz University of Antalya	TR
Pașc Gävrută, Prof.	Politehnic University of Timisoara	RO
Pavel Satrapa, Assoc. Prof.	Technical University of Liberec	CZ
Pavel Tvrdík, Prof.	Czech Technical University in Prague	CZ
Pavlina Yordanova, Assoc. Prof.	Shumen University	BG
Petr Trusov, Prof.	Perm State Technical University	RU
Rannveig Björnsdóttir, Prof.	University of Akureyri	IS
Roumen Anguelov, Prof.	University of Pretoria	ZA
Sándor Szabó, Dr. Prof.	University of Pécs	HU
Sashko Martinovski, Assoc. Prof.	St. Kliment Ohridski University of Bitola	MK
Sergey Bosnyakov, Prof.	Moscow Institute of Physics and Technology	RU
Sergey Kshevetskii, Prof.	Immanuel Kant Baltic Federal University	RU
Snejana Hristova, Prof.	University of Plovdiv	BG
Svetlana Lebed, Assoc. Prof.	Brest State Technical University	BY
Tomasz Szarek, Prof.	University of Gdansk	PL
Valeriy Serov, Prof.	University of Oulu	FI
Vasily Maximov, Prof.	Saint Petersburg State University of Industrial Technologies and Design	RU
Ventsi Rumchev, Prof.	Curtin University, Perth	AU
Veronika Stoffová, Prof.	University of Trnava	SK
Veselka Pavlova, Prof.	University of National and World Economy	BG
Viorica Sudacevschi, Assoc. Prof.	Technical University of Moldova	MD
Vladimir Janković, Prof.	University of Belgrade	RS
Vladislav Holodnov, Prof.	Saint Petersburg State Institute of Technology	RU
Vyacheslav Demidov, Prof.	Saint Petersburg State University of Industrial Technologies and Design	RU
Yordan Yordanov, Assoc. Prof.	University of Sofia	BG
Yuriy Kuznetsov, Prof.	Nizhny Novgorod State University	RU
Zdenka Kolar - Begović, Prof.	University of Osijek	HR

INTERNATIONAL SCIENTIFIC JOURNAL

MATHEMATICAL MODELING

PUBLISHER:

SCIENTIFIC TECHNICAL UNION OF MECHANICAL ENGINEERING
“INDUSTRY 4.0”

108, Rakovski Str., 1000 Sofia, Bulgaria

tel. (+359 2) 987 72 90,

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

office@stumejournals.com

www.stumejournals.com

ISSN (PRINT) 2535-0986

ISSN (WEB) 2603-2929

YEAR I, ISSUE 4 / 2017

EDITOR IN CHIEF:

Prof. D.Sc. ANDREY FIRSOV

Peter the Great St.Petersburg Polytechnic University, Russia

C O N T E N T S

THEORETICAL FOUNDATIONS AND SPECIFICITY OF MATHEMATICAL MODELLING

COMPARISON OF THE RESULTS OBTAINED BY PSEUDO RANDOM NUMBER GENERATOR BASED ON IRRATIONAL NUMBERS PhD. Dimitrievska Ristovska V., Prof. PhD. Bakeva V.	167
STATISTICAL METHODS FOR THE ANALYSIS OF THE MONTE CARLO SIMULATION RESULTS IN VISION SYSTEMS I. Yu. Gendrina, Ass. Prof., Ph.D.	171
MODELING OF LIQUID SPREADING IN RANDOMLY PACKED METAL PALL RINGS Dr. Petrova T., Stefanova, K., Dr. Dzhonova-Atanasova, D., Prof. Dr. Semkov, K.	174
A MATHEMATICAL MODEL OF VISCOUS LIQUID MIXTURE MOTION THROUGH A VERTICAL CYLINDRICAL PIPE Asst., MSc Sorokina Natalia	177

MATHEMATICAL MODELLING OF TECHNOLOGICAL PROCESSES AND SYSTEMS

COMPUTER SYSTEM FOR PREDICTING THE STRUCTURE AND PROPERTIES OF CAST METAL PRODUCTS Ass. Prof., Dr. Eng. Donii O., Ass. Prof., Dr. Eng. Kulinich A., Ass. Prof., Dr. Eng. Khristenko V.	180
DECISION OF OPTIMIZATION PROBLEMS USING SYMMETRIC ALGORITHM OF HEAVY BALL METHOD Kharlamova Y.N.	184
STABILITY ANALYSIS AND SIMULATIONS OF BIOREACTOR MODEL WITH DELAYED FEEDBACK Assist. Prof., Ph.D. Borisov M., Prof., Ph.D. Dimitrova N., Prof., D.Sc. Krastanov M.	188
INVESTIGATION OF SAMPLES ACCURACY TO MODEL THE PROCESSES IN 3D PRINTING Assoc. Prof. MEng. Minev R. PhD., Assoc. Prof. MEng. Rusev R. PhD., MEng. Antonov S. PhD., MEng. Minev E. PhD.	192
ELECTRIC POWER SYSTEMS MODELING AND EDUCATION: THE CONTROLLABLE LOADS IN A SHORT TERM SYSTEM BALANCE M.Sc. Trashlieva V., M.Sc. Radeva T. PhD.	196
NUMERICAL MODEL FOR SIMULATION OF THE VELOCITY FIELDS FOR THE EXPLOSIVELY FORMED PENETRATOR M.Sc. Hutov I. PhD., Prof. M.Sc. Lilov I. PhD.	199
MODELING OF PRODUCTION PARAMETERS OF B4C + ZrO2 COMPOSITES VIA ARTIFICIAL NEURAL NETWORKS METHOD S. Hartomacıoğlu. PhD., H.O.Gülsoy. PhD., B. Bakırcıoğlu Ms.C.	203

MATHEMATICAL MODELLING OF MEDICAL-BIOLOGICAL PROCESSES AND SYSTEMS

GENERATION OF AN ATLAS-BASED FINITE ELEMENT MODEL OF THE HEART FOR CARDIAC SIMULATION M.Sc. Vasiliev Evgeny	207
---	-----

COMPARISON OF THE RESULTS OBTAINED BY PSEUDO RANDOM NUMBER GENERATOR BASED ON IRRATIONAL NUMBERS

PhD. Dimitrievska Ristovska V., Prof. PhD. Bakeva V.

Faculty of Computer Science and Engineering- Ss. Cyril and Methodius University, Skopje, Macedonia,

vesna.dimitrievska.ristovska@finki.ukim.mk

verica.bakeva@finki.ukim.mk,

Abstract: Pseudo-random number generators (PRNG) based on irrational numbers are proposed elsewhere. They generate random numbers using digits of real numbers which decimal expansions neither terminate nor become periodic and practically their decimal expansion has infinite period. Using that algorithm, we generate sequences of random numbers and then we check their randomness with statistical tests from Diehard battery. Our main idea is to check if there is a difference in the randomness of the generated sequences if digits of any irrational non-transcendental number (like $\sqrt{2}, \sqrt{3}, \sqrt{5}, \dots$) are used versus the case when digits of a transcendental number (like π or e) are used. In our experiments we use about $3 \cdot 10^7$ digits of a given non-periodic irrational or transcendental number. Many experiments were done and all generated sequences by proposed PRNG based on irrational numbers passed the Diehard tests very well. We may conclude that there is not a significant difference in the randomness of the generated sequences in the both cases (irrational non-transcendental versus irrational transcendental number).

Keywords: PRNG, IRRATIONAL NUMBERS, TRANSCENDENTAL NUMBERS, STATISTICAL TESTS, DIEHARD BATTERY, RANDOMNESS

1. Introduction

Pseudo-random number generator (PRNG) is an algorithm which generates a long sequence of numbers $r_1, r_2, \dots$ which are elements of a given set of numbers and the distribution of generated numbers $r_1, r_2, \dots$ is supposed to be uniform.

A sequence of obtained random numbers $r_1, r_2, \dots$ should have two important properties: uniformity (i.e., they are equally probable everywhere) and independence (i.e., the current value of a random variable does not depend on the previous values).

In practice, we cannot construct an ideal PRNG, since the way we are building the mechanism is not a random one, but in fact it is completely determined by an initial value. This affects the uniformity and independence of the produced sequences and $r_1, r_2, \dots$ and that is why the word "pseudo" is used and we have to measure the randomness of the obtained sequences.

A good random number generator should have some additional qualities as large period and small order computational complexity.

This paper is organized as follows. In Section 2 we give a background and overview of related works. In Section 3 we explain basic ideas for construction of our generator of pseudo random numbers [2], basic principles for usage of statistical tests from Diehard battery and then we present the algorithm for the generator. The obtained results are given in Section 4. In Section 5, some conclusions are made.

2. Background and overview of related works

In this section we present some historical facts recall on L'Ecuyer (2017) in [4] about PRNGs which use irrational numbers.

The inspiration for using successive digits of π , e or any other transcendental number in order to generate a random number sequence is an old idea.

For example, Metropolis et al. (1950) in [6] succeeded to compute 2000 decimals of π and e and confirmed that these sequences pass elementary statistical tests. This testing was extended to the first 10000 decimals by Pathria (1962) in [7] and to 100000 decimals by Esmenjaud-Bonnardel (1965) in [3], and all of these sequences very well pass elementary statistical tests.

Till now, many sequences of digits of π have been obtained and tested and many papers have discussed this idea. The world record in 2016 was 22 459 157 718 361 decimal digits of π , computed in

about four months by Peter Trueb using an algorithm of Chudnovsky and Chudnovsky (1989) (in [1]), Bellard's formula, and the Y-Cruncher multi-threaded software (Yee, 2017) (in [9]). However, to give good reason that the successive digits of π (or any other given irrational number) in a given base b can be taken as random sequence, it should be good to know that this sequence of digits is uniformly distributed in base b , i.e., that each of the b possible digits appears with frequency $1/b$ (on average) in the infinite sequence. For π , practical counting over several digits suggests that this is true, but there is no known proof of it.

However, the property of uniform distribution of the digits of any given irrational number is not sufficient; we need to have the uniform distribution of the pairs, triplets, and so on.

In the latest years, there are some trials to design a PRNG using digits of any irrational number since irrational numbers have decimal expansions that neither terminate nor become periodic, practically their decimal expansion has infinite period. In [8], Rogers and al. (2015) proposed an algorithm for pseudo-random 5-digit numbers using the digits of π and made some visual and statistical analyses for goodness of proposed generator.

In [2], the author proposed a new algorithm for generating pseudo-random numbers using digits of any irrational number. The randomness of obtained sequences of numbers is checked by some statistical tests and the test results are very well.

In this our paper, the main work is: using algorithm proposed in [2], to check if there is a difference in the randomness of the generated sequences, if digits of any irrational non-transcendental number (like $\sqrt{2}, \sqrt{3}, \sqrt{5}, \dots$ or the golden ratio $\varphi = \frac{1+\sqrt{5}}{2}$) are used versus the case when digits of a transcendental number (like π or e) are used.

3. PRNG based on digits of irrational numbers

3.1 The main idea in the algorithm– n -tuples

We will explain the ideas for designing a PRNG using digits of an irrational number ([2]), by example digits of π . In this example, we will use sequential n -tuples, for example 10-tuples of digits from the decimal expansion of π . Using some database we will take l

digits of π . In the next step, decimal 10-digit number from every 10-tuple is generated.

If we take the obtained 10-digit *number* (which is obtained directly from the 10-tuple) then its value is in the range $0 \leq \text{number} < 10^{10}$ and we need to check if the *number* is greater than *max* (maximal allowed generated number). If it is true, we have to omit the obtained *number* and continue with checking the next 10-tuple. The 10-tuples are taken without overlapping.

But, we will improve the previous idea if we scale the obtained 10-digit *number* (which is obtained directly from the 10-tuple) from the range $0 \leq \text{number} < 10^{10}$ in the range $0 \leq \text{number} < 2^{32}$. In this way, there is no need to check if the scaled number is greater than *max*. Note that if the sequence of generated number is uniform then the scaled sequence will be uniform on the set $\{0, 1, \dots, \text{max}\}$.

These steps from the last idea will be repeated until we obtain *l* numbers.

3.2 Input parameters and the algorithm

In order to produce different sequences, each time when we started generating of a new sequence, we must initialize the beginning pointer to an arbitrary digit of the chosen irrational number. The position of the beginning pointer will be an input parameter. Also, the input parameter will be the length *n* of digits (*n*-tuples) for generating of each number in the sequence (in the previous example, we choose $n = 10$). Let stress that we compute the digits of any irrational number using package *Mathematica*.

Algorithm

[1] Choose an irrational number which digits will be used for generating random numbers.

[2] Set the length *n* of digits for generating of each number in the sequence, the position *s* of the beginning pointer (the first digit where the generating starts), the length *l* of generated sequence and the maximum *max* of the generated numbers.

[3] Let *counter*=0.

[4] Until *counter* ≤ *l* do

[4.1] Use slice size of *n* digits to generate a number *r*.

[4.2] Scale $r \leftarrow \left[\frac{r}{10^n - 1} \cdot \text{max} \right]$.

[4.3] Put pointer position $s \leftarrow s + n$.

[4.4] *counter* = *counter* + 1.

We will notice that software realization of this algorithm and many experiments were done using package *Mathematica*.

3.5. Diehard tests

Nowadays there are a lot of tests for randomness and all of them measure the difference between the generated pseudo-random sequences and the theoretically supposed ideal random sequence. We say that a PRNG passes a test if the random sequences produced by that PRNG pass the test with a probability near to 1. We can classify PRNGs depending of the tests they have passed. So, for obtaining a better classification we should have many different tests.

Over several years, George Marsaglia [5] has developed Diehard tests as a battery of statistical tests for measuring the quality of a random number generator. This battery was published in 1995. It consists of 15 statistical tests, and it is a comprehensive set of statistical tests for PRNG and serves as some kind of litmus for checking and certification of PRNG. If a PRNG passes Diehard statistical tests, then it can be used in deeper scientific researches.

The Diehard battery consists of Birthday Spacings Test, Overlapping 5-Permutation Test (OPERM-5), Binary rank tests, 31×31 Binary Matrix, 32×32 Binary Matrix, 6×8 Binary Matrix, Bitstream Test, Test OQSO (Overlapping quadruples sparse occupancy test), Test DNA, Count the 1's Test for specific bytes, Parking test, Minimum Distance Test, 3D Spheres Test, Squeeze Test, Overlapping Sums Test, Runs Test and Craps Test.

We will note that the most of the tests in Diehard return a *p*-value, which should be uniform on $[0, 1]$ if the input file contains truly independent random bits. Those *p*-values are obtained by $p = F(X)$, where *F* is the assumed cumulative distribution function of the sample (random variable *X*) – often normal. But that assumed *F* is just an asymptotic approximation, for which the fit will be worst in the tails. Therefore $p < 0.025$ or $p > 0.975$ means that the PRNG has "failed the test at the 0.05 level".

4. Results obtained from Diehard tests and discussion

Diehard tests have requirements with precise format of the numbers whose randomness they test. Explicitly, the file of the numbers should be a binary file of a hexadecimal integer nonnegative numbers with approximately 11 MB size. There should be ten numbers in each row, about 2 870 000 numbers in the file and the maximum number in the file should be $\text{max} = 2^{32} - 1$.

As we mentioned previously, some of Diehard tests give *p*-value, and some of them are performed several times and the result from these tests is the ratio of the number of passed tests and the total number of tests. Therefore, we presented the results in separated tables depends on the kind of test output.

In the next tables we will present some of the obtained results of Diehard tests applied to the sequences generated by our proposed algorithm in [2].

In Table 1, we present the percentage of passed Diehard test for 14 sequences generated by our PRNG using different irrational numbers or same irrational number with different initial pointer *s* or with different initial length *n*. The bold line in the table separates the sequences obtained from the digits of non-transcendent irrational numbers from them obtained from the digits of transcendent irrational numbers. Note that almost all sequences pass more than 90% of the Diehard test. Exception is only the sequence obtained using the digits from the $\sin 1$, where the percentage of passed tests is between 80% and 90%, but it is satisfactory.

Table 1 Success of Diehard tests

Irrational number	Seq. number	<i>n</i>	<i>s</i>	Time for sequence generation (in sec.)	Success of Diehard tests
ϕ	Seq. 1	10	1	630	91 %
$\sqrt{2}$	Seq. 2a	10	2	670	99 %
$\sqrt{2}$	Seq. 2b	10	1	678	98 %
$\sqrt{3}$	Seq. 3a	10	6	636	97 %
$\sqrt{3}$	Seq. 3b	12	2	653	92 %
$\sqrt{7}$	Seq. 4a	10	6	654	99 %
$\sqrt{7}$	Seq. 4b	10	3	662	91 %
$\sin 1$	Seq. 5a	10	2	351	85 %
$\sin 1$	Seq. 5b	10	4	478	87 %
$\sin 1$	Seq. 5c	9	4	529	86 %
π	Seq. 6	10	8	485	94 %
<i>e</i>	Seq. 7a	10	2	586	90 %
<i>e</i>	Seq. 7b	10	1	577	94 %
$\ln 2$	Seq. 8	10	3	627	95 %

In Table 2 and Table 3, we present the results from Diehard tests obtained from sequences generated from the digits of non-

transcendent numbers. In Table 2, we give the results of Diehard test which output is p -value and in Table 3, the results when the output is the ratio of the number of passed tests and the total number of tests. The red (bold) values in the tables mean that the sequence does not pass the corresponding test.

Table 2: Results from Diehard tests applied on the sequences generated by PGNG when irrational number is non-transcendental. Obtained p -values are presented

Seq. name	Seq. 1	Seq. 2a	Seq. 2b	Seq. 3a	Seq. 3b	Seq. 4a	Seq. 4b
Irr. number	φ	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{3}$	$\sqrt{3}$	$\sqrt{7}$	$\sqrt{7}$
	p -value						
Birthday Spacings test	0.10	0.87	0.37	0.40	0.23	0.15	0.34
OPERM-5	0.15 0.14	0.82 0.12	0.08 0.57	0.91 0.80	0.29 0.70	0.31 0.72	0.93 0.49
Binary-31 test	0.34	0.85	0.78	0.32	0.68	0.32	0.73
Binary-32 test	0.79	0.36	0.32	0.86	0.64	0.72	0.46
Binary-6x8 test	0.89	0.971	0.54	0.82	0.83	0.57	0.09
Count-Stream test	0.55 0.68	0.91 0.28	0.64 0.68	0.24 0.23	0.36 0.28	0.52 0.50	0.23 0.70
Parking test	0.48	0.30	0.73	0.30	0.18	0.38	0.977
Minim. Distance test	0.99	0.09	0.82	0.57	0.004	0.51	0.32
3D Spheres	0.88	0.96	0.74	0.92	0.28	0.47	0.15
Squeeze test	0.004	0.71	0.14	0.45	0.53	0.96	0.17
O-SUM test	0.42	0.31	0.50	0.03	0.30	0.48	0.26
Run test	0.12 0.80 0.39 0.86	0.85 0.69 0.19 0.27	0.96 0.14 0.34 0.61	0.12 0.02 0.82 0.40	0.47 0.68 0.78 0.40	0.80 0.52 0.87 0.91	0.65 0.31 0.82 0.56
Craps test	0.49 0.81	0.92 0.24	0.26 0.41	0.24 0.03	0.39 0.92	0.75 0.30	0.99 0.24

Table 3: Results from Diehard tests applied on the sequences generated by PGNG when irrational number is non-transcendental. No. of passed tests / No. of total tests are presented

Seq. name	Seq. 1	Seq. 2a	Seq. 2b	Seq. 3a	Seq. 3b	Seq. 4a	Seq. 4b
Irr. number	φ	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{3}$	$\sqrt{3}$	$\sqrt{7}$	$\sqrt{7}$
	No. of passed tests / total tests						
Bit stream test	20/20	19/20	20/20	19/20	20/20	20/20	20/20
OPSO	23/23	22/23	18/23	21/23	17/23	21/23	22/23
OQSO	26/28	28/28	28/28	28/28	25/28	25/28	28/28
DNA test	31/31	28/31	28/31	31/31	30/31	30/31	31/31
Count Bytes test	23/25	23/25	22/25	23/25	24/25	24/25	24/25

From the last two tables, we can conclude that the generated sequences passed almost all Diehard tests.

In Table 4 and Table 5, we present the results from Diehard tests obtained from sequences generated from the digits of transcendent irrational numbers.

Table 4: Results from Diehard tests applied on the sequences generated by PGNG when irrational number is transcendental. Obtained p -values are presented

Seq. name	Seq. 5a	Seq. 5b	Seq. 5c	Seq. 6	Seq. 7a	Seq. 7b	Seq. 8
Irr. number	$\sin 1$	$\sin 1$	$\sin 1$	π	e	e	$\ln 2$
	p -value						
Birthday Spacings test	0.40	0.05	0.17	0.56	0.03	0.08	0.24
OPERM-5	0.98 0.94	0.05 0.73	0.20 0.99	0.68 0.32	0.95 0.27	0.19 0.99	0.57 0.49
Binary-31 test	0.33	0.66	0.41	0.77	0.49	0.81	0.99
Binary-32 test	0.60	0.61	0.62	0.65	0.72	0.32	0.64
Binary-6x8 test	0.18	0.22	0.89	0.55	0.31	0.16	0.14
Count-Stream test	0.40 0.26	0.01 0.34	0.87 0.03	0.43 0.31	0.90 0.45	0.80 0.51	0.80 0.04
Parking test	0.006	0.19	0.98	0.71	0.27	0.34	0.69
Minim. Distance test	0.92	0.03	0.55	0.01	0.35	0.86	0.72
3D Spheres	0.49	0.09	0.99	0.86	0.78	0.46	0.15
Squeeze test	0.14	0.84	0.61	0.27	0.87	0.66	0.85
O-SUM test	0.99	0.003	0.36	0.31	0.61	0.52	0.82
Run test	0.53 0.08 0.97 0.52	0.25 0.93 0.39 0.013	0.76 0.34 0.84 0.21	0.10 0.61 0.13 0.73	0.42 0.74 0.97 0.48	0.36 0.28 0.39 0.71	0.25 0.65 0.44 0.51
Craps test	0.15 0.35	0.05 0.58	0.71 0.60	0.45 0.67	0.99 0.99	0.86 0.83	0.46 0.64

Table 5: Results from tests in Diehard battery, when irrational number is transcendental. Results are given with No. of passed tests / No. of total tests.

Seq. name	Seq. 5a	Seq. 5b	Seq. 5c	Seq. 6	Seq. 7a	Seq. 7b	Seq. 8
Irr. number	$\sin 1$	$\sin 1$	$\sin 1$	π	e	e	$\ln 2$
	No. of passed tests / total tests						
Bit stream test	19/20	19/20	19/20	16/20	18/20	20/20	19/20
OPSO	19/23	21/23	20/23	20/23	21/23	21/23	23/23
OQSO	27/28	28/28	25/28	28/28	27/28	27/28	24/28
DNA test	30/31	30/31	29/31	31/31	30/31	26/31	31/31
Count Bytes test	20/25	24/25	23/25	25/25	23/25	23/25	24/25

Analyzing the results from Table 4 and Table 5, we can conclude that the sequences generated from the digits of transcendent irrational numbers also passed almost all Diehard tests. As we concluded from Table 1, exception is only the sequence obtained using the digits from the $\sin 1$, where the results are a little

bit worse, but these sequences also passed more of the considered tests.

5. Conclusions

In this paper, we generate sequences using PRNG based on digits of different irrational numbers. Our goal is to check if the kind of irrational numbers (non-transcendent or transcendent) has influence to the randomness of generated sequences. Our expectations were that the transcendent numbers will give better results than non-transcendent ones, but the results reject our expectations. They confirm that almost all tested irrational numbers are good for using in our PRNGs and there is not a significant difference in the randomness of the generated sequences in the both cases.

Acknowledgements

This work was partially financed by the Faculty of Computer Science and Engineering at the "Ss. Cyril and Methodius" University in Skopje.

References

1. Chudnovsky D., G. Chudnovsky The computation of classical constants, in: Proceedings of the National Academy of Sciences of the USA 86, 1989, pp. 8178--8182
2. Dimitrievska Ristovska, V. Pseudo random generator based on irrational numbers, in: Trajanov D., V. Bakeva (eds.): ICT-Innovations 2017, Data Driven Innovations, Conference Web Proceedings, 2017, pp. 105--113
3. Esmenjaud-Bonnardel M. Étude Statistique des Décimales de Pi, Revue Francaise de Techniques Informatiques 8 (4), 1965, pp. 295--306
4. L'Ecuyer P. History of uniform random number generation, Chan W. K. V., D'Ambrogio A., Zacharewicz G., Mustafee N., Wainer G., and Page E., eds.: DIRO, GERAD, and CIRRELT, Proceedings of the 2017 Winter Simulation Conference, 2017
5. Marsaglia G., W. W. Tsang Some difficult-to-pass tests of randomness, Journal of Statistical Software, Volume 7, Issue 3, 2002
6. Metropolis N., G. Reitwiesner, J. von Neumann Statistical Treatment of Values of First 2000 Decimals Digits of E and Pi Calculated on the ENIAC, Mathematical Tables and Other Aids to Computation 4, 1950
7. Pathria R. K. A Statistical study of randomness among the first 10000 digits of Pi, Mathematics of Computation 16, 1962, pp. 188--197
8. Rogers I., G. Harrell, J. Wang Using Pi digits to generate random numbers: A Visual and statistical analysis, Int'l Conf. Scientific computing | CSC'15 |
9. Yee A. J. Y-Cruncher—A Multi-Threaded Pi-Program, 2017

STATISTICAL METHODS FOR THE ANALYSIS OF THE MONTE CARLO SIMULATION RESULTS IN VISION SYSTEMS

I. Yu. Gendrina, Ass. Prof., Ph.D.
National Research Tomsk State University, Tomsk, Russia
igendrina@bk.ru

Abstract: In this paper, we present some results of statistical processing of the results of numerical simulation of the characteristics of vision systems through the atmosphere obtained with the help of a special software package created by us (Gendrina I.Yu., Kvach A.S.).

Keywords: Vision system, angular brightness distribution, Monte Carlo method, regression.

Introduction

Various methods of statistical research such as correlation-regression analysis, dynamic series, variance analysis, etc. in the study of vision systems are used for studying and subsequent prediction of the patterns of radiation transfer. We have conducted Monte Carlo experiments to calculate the Point Spread Function for linear system "underlying surface – atmosphere". The one is defined as the system response to the input signal, representing a point mass, located at a certain point, and can be determined as the angular brightness distribution of surface-based point source measured with receiving device at the top of the atmosphere. Then we have attempted to apply elements of correlation-regression analysis for the study of the influence of various optical and geometrical parameters on the Point Spread Function.

Vision system (VS) is understood as an observation scheme including the underlying surface, a "cloudy environment" (atmosphere), and an optical device that captures incoming radiation. To study radiation transfer in such systems, the theory of systems and the theory of radiation transfer are traditionally used (Zuev V.E., Belov V.V., Veretennikov V.V.).

The main system characteristic for VS is the point spread function (PSF); it is defined as the response L of linear system to the input signal, representing a point mass $\delta(x - x_1)\delta(y - y_1)$, located at a certain point (x_1, y_1) : $L[\delta(x - x_1)\delta(y - y_1)] = h(x, y; x_1, y_1)$.

An arbitrary object (function) $f(x, y)$ can be considered as a set of point masses. For instance:

$$f(x, y) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(x_1, y_1) \delta(x - x_1, y - y_1) dx_1 dy_1. \quad \text{Then, a}$$

result of the system impact (image) can be represented in the form:

$$g(x, y) = L[f(x, y)] = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(x_1, y_1) h(x, y; x_1, y_1) dx_1 dy_1.$$

Obviously, regularities of the image distortion due to impact of any system can be studied by analyzing the effect of this system on the point spread function.

The model of the atmosphere includes the following characteristics: the total attenuation coefficient $\sigma(\lambda, \vec{r}) = \sigma_{sc}(\lambda, \vec{r}) + \sigma_a(\lambda, \vec{r})$, where σ_{sc} – the scattering coefficient, σ_a – the absorption coefficient; $g(\lambda, \mu, \vec{r})$ – aerosol phase function. Here $\vec{r} = (x, y, z)$ – radius-vector of the current point in space, $\mu(\vec{\omega}', \vec{\omega})$ – cosine of the scattering angle of radiation coming from direction $\vec{\omega}'$, in the direction $\vec{\omega}$, λ – is the wavelength of incident radiation.

The paper considers two models of the atmosphere:

1. vertically bounded plane-parallel layer-homogeneous aerosol-molecular;

2. vertically bounded plane-parallel aerosol-molecular, including overcast layer. For the cloud layer, different characteristics from those of the first model is assumed: coefficients of attenuation, absorption, scattering, and the aerosol phase function.

1. Problem Statement and methods

The geometric scheme of calculations is as follows: at the lower boundary of the atmosphere (on the underlying surface $z = 0$) there is a point source of unit capacity. At the upper boundary of the atmosphere ($z = 30 \text{ km}$) there is an optical receiver that can receive scattered radiation coming from different directions (observation angles). The brightness of the scattered radiation is solution of the integro-differential transport equation (Marchuk G.I., Mikhailiov G.A., Nazaraliev M.A., Darbinjan, Kargin B.A., Elepov B.S.), which can be practically solved only by approximate or numerical methods.

One of the most universal methods for solving this problem is the simulation method, or the Monte Carlo method. The basis of the Monte Carlo method is the integral transport equation of the second kind with a generalized kernel for the density of particles' collisions (Marchuk G.I., Mikhailiov G.A., Nazaraliev M.A., Darbinjan, Kargin B.A., Elepov B.S.):

$$f(\vec{x}) = \int_{\vec{x}} k(\vec{x}', \vec{x}) f(\vec{x}') d\vec{x}' + \psi(\vec{x}), \quad f = Kf + \psi$$

Here $\vec{x} = (\vec{r}, \vec{\omega})$ – is the point of the phase space of coordinates and directions, $\psi(\vec{x})$ – source function, K – integral operator with kernel $k(\vec{x}', \vec{x})$:

$$k(\vec{x}', \vec{x}) = \frac{\sigma_{sc}(\vec{r}) \cdot g(\mu) \exp(-\tau(\vec{r}', \vec{r})) \sigma(\vec{r})}{\sigma(\vec{r}') 2\pi |\vec{r} - \vec{r}'|^2} \cdot \delta\left(\vec{\omega} - \frac{\vec{r} - \vec{r}'}{|\vec{r} - \vec{r}'|}\right)$$

In this paper, one of the algorithms of the Monte Carlo method was used - the method of local estimation (Marchuk G.I., Mikhailiov G.A., Nazaraliev M.A., Darbinjan, Kargin B.A., Elepov B.S.).

Algorithm for local estimation consists in calculating following functional:

$$J(\Omega_i) = \int_{\Omega_i} \Phi(\vec{r}^*, \vec{\omega}^*) d\vec{\omega}^* = \int_{\vec{x}} l_i(\vec{x}, \vec{x}^*) f(\vec{x}') d\vec{x}' = \quad (1)$$

$$= M \sum_{n=0}^N Q_n \cdot l_i(\vec{x}_n, \vec{x}^*)$$

$$l_i(\vec{x}, \vec{x}^*) = \frac{\exp(-\tau(\vec{r}, \vec{r}^*)) \cdot g(\mu^*)}{2\pi |\vec{r} - \vec{r}^*|^2} \Delta_i(\vec{s}^*). \quad (2)$$

$$\text{Here } \vec{s}^* = \frac{\vec{r}^* - \vec{r}}{|\vec{r}^* - \vec{r}|}, \quad \mu^* = (\vec{\omega}, \vec{s}^*), \quad \Delta_i(\vec{s}) - \text{ is}$$

the indicator of region Ω_i . Φ – flux of particles at given point $\vec{x}^*$. Q_n – weight of the particle, $f(\vec{x})$ – density of collisions.

2. Initial data

We will consider the process of radiative transfer through aerosol-molecular atmosphere, which comprises a layer overcast, by neglecting the reflection from underlying surface. We used the following data (Gendrina I.Yu., Kvach A.S.):

1. Wavelength (mkm) in transparent windows: 0.347; 0.530; 0.694; 0.860; 1.060; 3.390; 10.60.

2. Lower boundary of atmosphere 0 km above Earth's surface, upper boundary H of the atmosphere 30 km above the Earth's surface.

3. Optical thickness for a cloudless atmosphere are presented in Table 1.

Table 1. Optical thickness of the cloudless atmosphere

Wavelength, mkm	Optical thickness
0,347	0,228
0,53	0,158
0,694	0,124
0,86	0,098
1,06	0,092
3,39	0,067
10,6	0,041

4. Lower boundary of the cloud layer - 1 km above the Earth's surface, upper boundary - 2 km above the Earth's surface. The optical models of the cloud layer – “haze H” and “cloud C1” (Deirmendjian D.)

5. In this work, we considered Lambertian model of sources of radiation. In this case the density of the initial areas

looks like: $p(\vec{\omega}) = \frac{\mu}{\pi}$, where $\mu = \arccos \theta$, θ - zenith angle of initial direction.

3. Simulation results

Quantitative values brightness of scattered radiation for the cloudless atmosphere are presented in our previous publication (Gendrina I.Yu., Alekseenko M. A.). Similar values for various models of the cloud atmosphere are given in Tables 2,3.

Table 2 contains the results for the brightness of scattered radiation for the atmosphere with a cloud layer of the “Haze H” type.

Table 3 contains similar data for the atmosphere with a cloud layer of the “Cloud C1” type.

These types vary in value of the average cosine of scattering phase function:

$$\bar{\mu} = \frac{1}{2} \int_{-1}^1 \mu g(\mu) d\mu.$$

It is known that this parameter characterizes the elongation of aerosol phase function. For example in case $\lambda = 0,694$ mkm the average cosine amounts to 0,745 for type “Haze H” and 0,857 for type “Cloud C1”.

Table 2. Brightness of scattered radiation for the atmosphere with a cloud layer of the “Haze H” type, $W/mkm \cdot m^2$

Angles of reception, grad	Wavelength, mkm			
	$\lambda=0,374$	$\lambda=0,530$	$\lambda=0,694$	$\lambda=0,860$
4,5	2,24E-05	1,67E-05	1,38E-05	1,13E-05
13,5	1,09E-06	7,65E-07	6,60E-07	5,30E-07
22,5	2,23E-07	1,83E-07	1,55E-07	1,39E-07

31,5	8,44E-08	5,63E-08	5,54E-08	4,73E-08
40,5	3,49E-08	2,73E-08	2,81E-08	6,65E-08
49,5	1,86E-08	5,15E-08	1,54E-08	1,18E-08
58,5	1,30E-08	1,10E-08	1,71E-08	7,75E-09
67,5	1,94E-08	1,12E-08	7,95E-09	2,11E-08
76,5	1,58E-07	2,13E-08	4,96E-09	3,68E-09
85,5	1,20E-08	6,37E-09	1,23E-09	1,03E-09

Table 3. Brightness of scattered radiation for the atmosphere with a cloud layer of the “Cloud C1” type, isotropic source, $W/mkm \cdot m^2$

Angles of reception, grad	Wavelength, mkm			
	$\lambda=0,374$	$\lambda=0,530$	$\lambda=0,694$	$\lambda=0,860$
4,5	4,24E-07	5,01E-07	5,45E-07	5,69E-07
13,5	1,32E-07	1,36E-07	1,01E-07	9,47E-08
22,5	5,06E-08	4,30E-08	4,23E-08	3,50E-08
31,5	2,29E-08	1,84E-08	1,20E-08	1,19E-08
40,5	7,00E-09	8,43E-09	6,45E-09	5,16E-09
49,5	3,29E-09	2,44E-09	3,10E-09	2,69E-09
58,5	1,84E-09	1,59E-09	1,36E-09	1,39E-09
67,5	1,17E-09	1,13E-09	7,77E-10	8,25E-10
76,5	8,77E-10	9,73E-10	7,45E-10	5,32E-10
85,5	1,70E-10	5,77E-10	8,95E-11	1,78E-10

4. Statistical analysis of simulation results

To establish functional relationship between the angular distribution of brightness and optical parameters, regression analysis was used, which is widely used to restore aerosol and cloud characteristics, and also to assess their effect on climate (Khayer M. M. et al.). The regression equation for the angular distribution of brightness in the aerosol-molecular and cloud atmosphere relatively wavelength of the incident radiation was

obtained in the form $y = \frac{b_1}{x} + b_0$ for all reception angles.

Regression coefficients for the cloudless atmosphere are given in Table 4. The regression coefficients for the cloudy atmosphere are given in Table 5. The tables also shown coefficients of determination R^2 . This coefficient indicates the proportion of the total variation in the dependent variable y due to variability of x and characterizes the total quality of regression. The statistical significance of determination coefficient can be

confirmed with the help of Fisher statistics: $F = \frac{R^2}{1 - R^2} \cdot (n - 2)$.

Here n is the number of observations. The value F is compared to value $F_{\alpha; k_1, k_2}$ from Fisher table. Here α - the given level of significance, $k_1 = 1$ and $k_2 = n - 2$.

Table 4. Coefficients of the regression equation for the cloudless atmosphere

Angles of reception, grad	b_0	b_1	R^2
4,5	1,19E-05	3,25E-05	0,993
13,5	2,31E-07	5,05E-07	0,976
22,5	6,98E-08	1,19E-07	0,927
31,5	3,92E-08	4,04E-08	0,784
40,5	2,44E-08	1,51E-08	0,570
49,5	1,39E-08	6,51E-09*	0,482
58,5	6,82E-09	3,64E-09	0,609
67,5	2,74E-09	2,35E-09	0,771
76,5	5,21E-10	1,23E-09	0,907
85,5	3,00E-11	1,76E-10	0,929

Table 5 Coefficients of the regression equation for the cloud atmosphere

Angles of reception, grad	b_0	b_1	R^2
4,5	3,52E-06	7,12E-06	0,985
13,5	1,08E-07	3,63E-07	0,997
22,5	3,63E-08	7,53E-08	0,973
31,5	1,26E-08	2,66E-08	0,976
58,5	3,68E-09*	4,34E-09	0,598
76,5	-3,34E-08*	5,04E-09	0,606
85,5	-2,37E-09*	4,50E-09	0,809

We would like to present also the brightness dependence relatively the upper boundary of cloud. The regression equation in this case was obtained in a simple form: $y = b_1x + b_0$ for all reception angles. Regression coefficients and determination coefficients for the case of isotropic source, wavelength of $\lambda = 0,347$ mkm, cloud layer type of the "Haze H" and "Cloud C1" are given in Table 6,7.

Table 6. Coefficients of the regression equation for the cloud atmosphere. Model «Haze H»

Angles of reception, grad	b_0	b_1	R^2
4,5	5,14E-07	-3,07E-08	0,990
13,5	1,53E-07	-7,70E-09	0,975
22,5	5,92E-08	-2,33E-09	0,851
31,5	2,65E-08	-6,54E-10*	0,654
40,5	7,36E-09	-1,75E-10	0,946
49,5	3,60E-09	-6,36E-11	0,625
58,5	2,11E-09	-5,13E-11	0,840
67,5	1,25E-09	-2,96E-11	0,886

Table 7. Coefficients of the regression equation for the cloud atmosphere Model «Cloud C1»

Angles of reception, grad	b_0	b_1	R^2
4,5	4,98E-07	-2,61E-08	0,966
13,5	1,44E-07	-4,88E-09	0,953
22,5	5,10E-08	-1,48E-10	0,158
31,5	2,14E-08	7,33E-10	0,976
40,5	6,30E-09	1,55E-10*	0,631
49,5	3,15E-09	4,54E-11	0,882
58,5	1,89E-09	-8,70E-12*	0,379
67,5	1,18E-09	-7,32E-12	0,802
76,5	1,11E-09	2,66E-11*	0,151

Note. * - insignificant coefficient.

Conclusions

Statistical estimation of regression equations for significance was carried out on the basis of the F -test and estimation of the determination coefficient. With 90% confidence, it can be argued that the considered dependence is statistically significant.

The analysis shows that between obtained angular distributions of intensity and wavelength) in transparent windows for both cloudless and cloudy for the atmosphere, there is a link that can be with a good degree of accuracy to describe hyperbolic regression equation.

Between the brightness and the upper boundary of cloud, there is a link that can be with a degree of accuracy to describe linear regression equation.

References

1. Gendrina I.Yu., Kvach A.S., "The Monte Carlo method for determining the vision system characteristics", J. of International Scientific Publication: Education Alternatives, 11(1), 236 – 244 (2013).
2. Zuev V.E., Belov V.V., Veretennikov V.V., [Systems with applications in scattering media], Publishing House "Spectrum" Institute of Atmospheric Optics of the Siberian Branch of the Russian Academy of Sciences, 157-168 (1997).
3. Marchuk G.I., Mikhailiov G.A., Nazaraliev M.A., Darbinjan, Kargin B.A., Elepov B.S., [The Monte Carlo method in atmospheric optics], Nauka, Novosibirsk, 4-95 (1976).
4. Deirmendjian D., [Electromagnetic scattering on spherical polydispersions], American Elsevier Pub. Co., 1-290 (1969).
5. Gendrina I.Yu., Alekseenko M. A., "The regression analysis of statistical simulation results in vision systems through the atmosphere", Izvestija-vuzov-fizika, 58 (8/2), 294-296 (2015).
6. Khayer M. M. et al., "Evaluation of a 5-Year Cloud and Radiative Property Dataset Derived from GOES-8 Data Over the Southern Great Plains", Twelfth ARM Science Team Meeting Proceedings, 1-14 (2002).

MODELING OF LIQUID SPREADING IN RANDOMLY PACKED METAL PALL RINGS

МОДЕЛИРАНЕ НА РАЗТИЧАНЕТО В НЕНАРЕДЕНИ МЕТАЛНИ ПРЪСТЕНИ НА ПАЛ

Dr. Petrova T., Stefanova, K., Dr. Dzhonova-Atanasova, D., Prof. Dr. Semkov, K.

Bulgarian Academy of Sciences, Institute of Chemical Engineering
Akad. G. Bonchev Str., bl.103, 1113 Sofia, Bulgaria,

e-mail: tancho66@yahoo.com

Abstract: The present work compares two different approaches, Computational Fluid Dynamics (CFD) and dispersion model, for liquid distribution modeling with experimental data for liquid spreading in randomly packed metal Pall rings. The used experimental data are obtained in a semi-industrial column with a 0.6m diameter for several packing heights and liquid loads. It is shown that the appropriate choice of dispersion model parameters is essential for prediction of liquid distribution. In both models some parameters are determined by fitting with experimental data, the remainder are calculated or taken from literature. Comparison of the two model liquid distributions with experimental data shows that both CFD and dispersion model are in good agreement with the experiment especially for higher packing bed, when the wall flow is fully developed.

Keywords: PACKED-BED COLUMN, LIQUID DISTRIBUTION, RANDOM PACKING, DISPERSION MODEL, PARAMETER IDENTIFICATION

1. Introduction

Packed columns are widely used for separation processes such as rectification and absorption in chemical industry and environmental protection due to their high efficiency at low pressure drop. The recent interest is connected with technologies for flue gas scrubbing, heat recovery and fuel production. The uniform liquid distribution in the packed bed cross-section is crucial for the efficiency of the transfer processes. Several models are proposed to predict the liquid distribution in a packed bed starting from the random walk model of Tour and Lerman [1] for liquid spreading in unconfined packing with no wall effect and the dispersion model of Cihla and Schmidt [2] developed by other authors to account for the wall flow. Lately the techniques of Computational Fluid Dynamics (CFD) are widely employed for prediction of the liquid distribution by treating the packing bed as a porous media with permeability resistance, Yin [3], or by reconstructing the geometry of the packing bed and tracking the gas-liquid interface area.

The present work compares results from a dispersion model and a CFD simulation of liquid spreading in a packed bed of random Pall rings.

2. Model description

In this part a brief concept of dispersion model equations, boundary conditions, and solution is presented. The full description is given in the work [4]. The process of flow distribution in a packed-bed column is described by the following dimensionless equation [2]:

$$(1) \left(\frac{\partial^2 f(r, z)}{\partial r^2} + \frac{1}{r} \frac{\partial f(r, z)}{\partial r} \right) = \frac{\partial f(r, z)}{\partial z},$$

where $r = r'/R$ is dimensionless radial coordinate; r' is radial coordinate, m; R is column radius, m; $z = Dh/R^2$ is dimensionless axial coordinate; D is liquid distribution coefficient, m; h is axial coordinate, m; $f = L/L_0$ is dimensionless superficial velocity; L, L_0 are local and mean liquid superficial velocity, $m^3/m^2 \cdot s$. The boundary conditions are the following [5]:

$$(2) -\frac{\partial f}{\partial r} = B(f - CW), \quad \text{for } r = 1$$

$$(3) \frac{\partial f(r, z)}{\partial r} = 0, \quad \text{for } r = 0$$

where parameter B is a criterion for exchange of liquid between the column wall and the packing; parameter C expresses the equilibrium distribution of entire liquid flow between the wall and the packing when equilibrium state is attained $z \rightarrow \infty$; W is dimensionless wall flow.

The equations defining these parameters are:

$$(4) B = \beta R / D,$$

$$(5) C = \pi R^2 \gamma,$$

where β , $-$, and γ , $1/m^2$, are parameters in the boundary conditions.

At $z = 0$ the uniform initial irrigation is defined as:

$$(6) f(r, z) = 1, \text{ for } 0 \leq r < 1 \text{ and } z = 0$$

There is analytical solution of the above model in the form of infinite series [6]:

$$(7) f^u(r, z) = A_0 + \sum_{n=1}^{\infty} A_n^u J_0(q_n r) \exp(-q_n^2 z),$$

In the above expressions, f^u (dimensionless), denotes the solution for uniform initial irrigation. The coefficients are derived from the expressions:

$$(8) A_0 = \frac{C}{1+C}, \quad A_n^u = \frac{2(q_n^2 / B - 2C)}{\left[(q_n^2 / B - 2C)^2 + q_n^2 + 4C \right] J_0(q_n)},$$

The dimensionless wall flow W^u is calculated from Eq. (9) and from the material balance:

$$(9) W^u = \frac{1}{1+C} - 2 \sum_{n=1}^{\infty} A_n^u(q_n) \frac{J_1(q_n)}{q_n} \exp(-q_n^2 z),$$

where J_0, J_1 are Bessel functions of the first kind, zero and first order; q_n are the roots of the characteristic equation, following from boundary condition (2):

$$(10) [(2C/q_n) - (q_n/B)] J_1(q_n) + J_0(q_n) = 0$$

3. Experimental data.

Experimental data for the liquid distribution in a column filled with metal Pall rings, of 25 mm, used in this paper are taken from the PhD thesis of Yin [3]. They are obtained in a pilot column with 0.6m diameter, for packing heights 0.9 and 3.0 m, and liquid and gas loads $L = 2.91; 4.78; 6.66, G = 0; 0.75 \text{ kg/m}^2 \cdot \text{s}$. The liquid collecting device consists of 6 segments, the initial irrigation is uniform.

4. Methods of estimation and identification of model parameters

In this paper we propose the following scheme for three parameters' estimation/identification of the mathematical model described above.

1) The value of C can be determined even if there are not available data for wall initial irrigation. In this case the data about wall flow at several packing heights for uniform initial irrigation are needed. We use the relation (9) in the limiting case when $z \rightarrow \infty$; as it is seen, the last term in (9) diminishes and the result is:

$$(11) W^u \Big|_{z \rightarrow \infty} = \frac{1}{1+C},$$

2) In this work the value of the radial spreading coefficient D is taken from the literature [7];

3) Then, only parameter B can be identified by non-linear optimization minimizing the residual variance:

$$(12) S_A^2 = \frac{1}{k-1} \sum_{i=1}^k n_i (f_{ie} - f_{ic})^2,$$

where f_i is the mean dimensionless density of irrigation in i -th annular section of the liquid collecting device, delimited by the radii r_{i-1} and r_i ($r_i > r_{i-1}$) and is determined by the expression

$$(13) f_i = \frac{2}{r_i^2 - r_{i-1}^2} \int_{r_{i-1}}^{r_i} f(r, z) r dr,$$

with indices "e" and "c" denoting experimental and calculated values of liquid density of irrigation.

As explained above, three parameters should to be determined – C, D and B . In the light of experimental data used in this paper, for calculation of C eq. (11) is used. Then, the obtained value for C is 5.95, which is very close to the value ($C = 5.29$), obtained for ceramic Pall rings 25 mm in [4]. Here, the value of C is calculated from the results [3] for the wall flow at uniform initial irrigation for packing heights 0.9, 1.8 and 3.0 m at liquid load $L = 6.66 \text{ kg/m}^2 \cdot \text{s}$ and no gas flow, because at these conditions a fully developed wall flow is achieved. As it is recommended in [8], the value of C is better to obtain from data at higher packing layer, when the equilibrium between bulk zone and wall flow is reached. On the contrary, these authors mentioned, that the parameter B has to be identified/calculated

for lower packing depths, because at higher ones it loses its importance.

In this work the value of D is chosen to be $D = 0.0007 \text{ m}$. This value is the last result [7], reported in the literature about metal Pall rings, 25.4 mm, and, which is more important, the results of Wen et al.[7] are obtained for the same packing, as in [3]. The previous reported data for D is that of Stikkelmann [9], which is about 3 times larger (0.0025m) although the method of calculating of D is the same as in the work [7]. The probable explanation of these differences in the value of D is that a piece of Pall ring packing may have different geometry inside its cylindrical body – see [10]. The Pall rings are created in 1940 and up to now a large number of manufacturers as well as many modifications of this packing type exist (Flexiring, Raflux ring, P-ring, Hy-pak, etc.). The cut "windows" in one packing element may have different width and curvature, which changes the radial spreading inside the packing element, and this result in a large variety of spreading coefficients even for the same packing diameter and material [11]. In [4], the reported value for ceramic Pall rings, 25 mm, for approximate comparison, is $D = 0.0011 \text{ m}$, but the inside geometry of ceramic Pall rings is different from that of metal one.

The only one model parameter to be identified is B . That is done using the minimal residual variance (12) between model and experimental mean dimensionless density of irrigation (13) in each segment of liquid collecting device (detailed procedure is described in [12]. The obtained value is $B = 25$.

4. Comparison of liquid predictions (CFD results of Yin [3] and current model) with experimental data for metal Pall rings [3]

In [3], the comparison between experimental and CFD data for liquid relative velocity is made, for packing heights $H=0.9 \text{ m}$ and $H=3.0 \text{ m}$, for $L=4.78 \text{ kg/m}^2 \cdot \text{s}$ and $G=0.75 \text{ kg/m}^2 \cdot \text{s}$, which is below the reported loading point and the influence of the gas phase is not significant. We compare these results with model solution (7) for already identified values of the parameters. The comparison of both model predictions - CFD and dispersion model from this work are presented in figures 1 and 2.

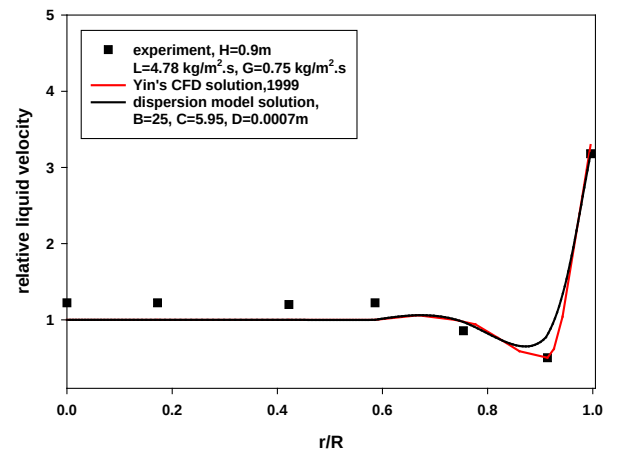


Fig. 1 Comparison of relative liquid velocities between dispersion model predictions, Yin's CFD predictions and Yin's experimental data: $L=4.78 \text{ kg/m}^2 \cdot \text{s}$; $G=0.75 \text{ kg/m}^2 \cdot \text{s}$; for packing height $H=0.9 \text{ m}$.

As can be seen, both models describe very well experimental data. For lower packing height the radial profile of experimental data in the bulk zone are still parabolic and equalize when the packing height is increased. Both predictions are more accurate at $H=3.0 \text{ m}$.

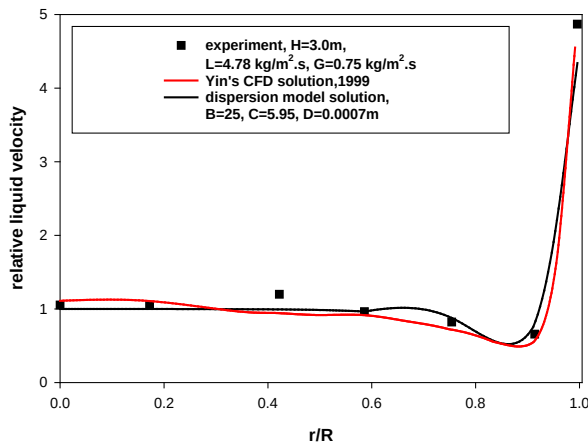


Fig. 2 Comparison of relative liquid velocities between dispersion model predictions, Yin's CFD predictions and Yin's experimental data: $L=4.78 \text{ kg/m}^2\text{s}$; $G=0.75 \text{ kg/m}^2\text{s}$; for packing height $H=3.0 \text{ m}$.

It should be mentioned, that at both figures, model predictions of [3] are performed with the aid of the modern CFD package CFX4.2. Two of the parameters, included in the closure equations and relations, also were obtained by fitting with the experiment. They are connected with 'liquid dispersion coefficient', defined by Yin [3] for volume average concept, and turbulent term, included in it.

In the case of no gas flow, in the next figures 3 and 4, the results of dispersion model predictions for the same heights, but for different liquid loads $L=2.91 \text{ kg/m}^2\text{s}$ and $L=6.66 \text{ kg/m}^2\text{s}$ are also presented. For above identified model parameters the coincidence between the model and experiment is quite well, which is additional verification of dispersion model ability to predict liquid spreading in packed beds.

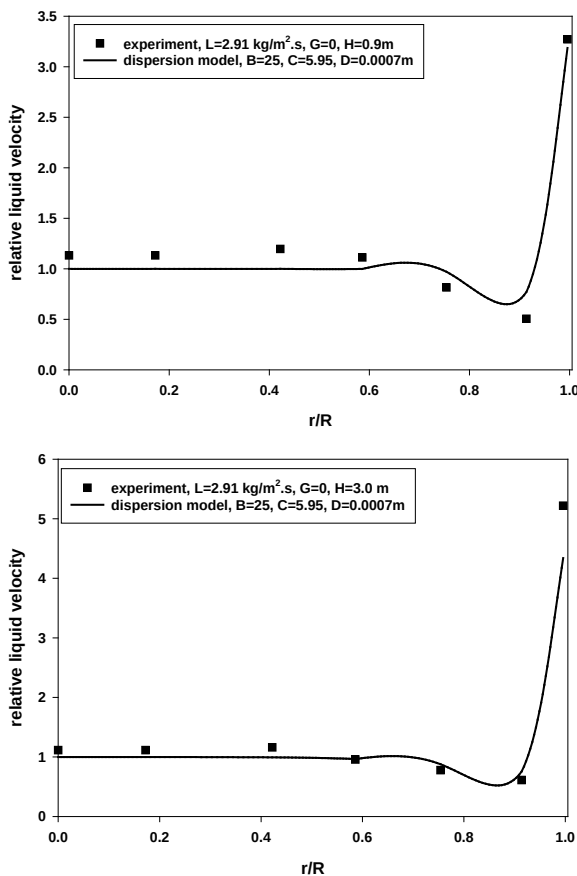


Fig. 3 Comparison of relative liquid velocities between dispersion model predictions and Yin's experiment: $L=2.91 \text{ kg/m}^2\text{s}$; $G=0$; for packing heights $H=0.9\text{m}$ (up) and $H=3.0\text{m}$ (down).

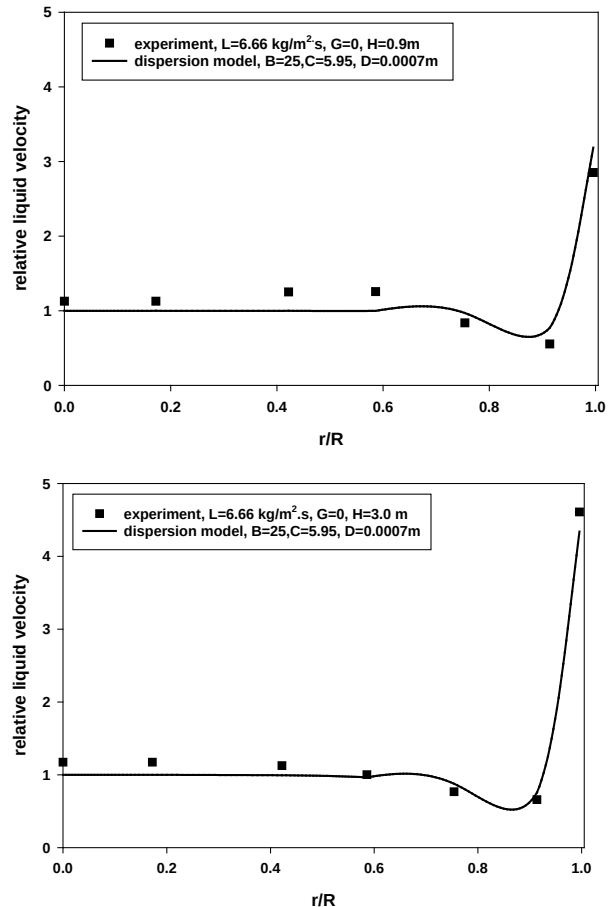


Fig. 4 Comparison of relative liquid velocities between dispersion model predictions and Yin's experiment: $L=6.66 \text{ kg/m}^2\text{s}$; $G=0$; for packing heights $H=0.9\text{m}$ (up) and $H=3.0\text{m}$ (down).

5. Conclusions

In the current work the results of dispersion model prediction for liquid distribution in random packing and identification procedure for model parameters are presented. A new formula is proposed for estimation of model parameter C in the case of uniform initial irrigation only, and experimental data for liquid distribution at several packing layer heights. Validation of model prediction for identified model parameters with experimental data of [3] for Pall rings, at two different packing heights and three liquid loads shows, that dispersion model analytical solution could be used successfully for fast prediction of liquid distribution in randomly packed beds.

The dispersion model results are also compared with CFD prediction and experimental data of Yin for liquid distribution in a packed bed with metal Pall rings [3]. Comparison of two theoretical liquid distributions with experimental one show, that both describe very well the experimental data.

6. Literature

1. Tour, R. S. , F. Lerman. Unconfined distribution of liquid in tower packing, Trans. AICHE 35, 1939, 709-718
2. Cihla, Z., O. Schmidt. A study of the flow of liquid when freely trickling over the packing in a cylindrical tower. - Collect. Czech. Chem. Commun., 22, 1957, 896-907
3. Yin, F., Liquid maldistribution and mass transfer efficiency in randomly packed distillation columns, PhD thesis, Department of chemical and material engineering, University of Alberta, Edmonton, Alberta, Canada, 1999.

4. Semkov, Kr., T. Petrova, P. Moravec. Parameters Identification of a Mathematical Model for Liquid Distribution in Packed-Bed Columns. - Bulgarian Chemical Communications, 32, 3-4, 2000, 497 – 516
5. Staněk, V., V. Kolář. Distribution of liquid over random packing. - Collect. Czech. Chem. Commun., 30, 1965, 1054-1059
6. Staněk, V., V. Kolář. Distribution of liquid over a random packing . VIII Distribution of the density of wetting in a packing for an arbitrary type of initial conditions. - Collect. Czech. Chem. Commun., 38, 1973, 2865-2873
7. Wen, X., Y. Shu, K. Nandakumar, K. Chuang. Predicting Liquid Flow Profile in Randomly Packed Beds from Computer Simulation. - AIChE Journal, 47, 8, 2001, 1770-177
8. Staněk, V., V. Kolář. Distribution of liquid over a random packing: Verification of the boundary condition of liquid transfer between a packed bed and the wall of a cylindrical column and evaluation of its parameters. - Collect. Czech. Chem. Commun., 33, 4, 1968, 1062-1077
9. Stikkelmann, R. Gas and liquid maldistributions in packed columns. - PhD thesis, Technical University of Delft, Delft, Netherlands, 1989
10. Web brochure : <http://www.rubbersealing.com/TCI/category-34-b0--Random+Tower+packing-pall+ringHiflow+ring.html>
11. Petrova, T., Kr. Semkov, S. Darakchiev, R. Darakchiev. Разтичане на течността в колони с ненаредени пълнежи. - Научни трудове на УХТ –Пловдив, 56, 2, 2009, 245 – 250
12. Dzhonova-Atanasova, D., Kr. Semkov, T. Petrova, S. Darakchiev, K. Stefanova, Sv. Nakov, R. Popov. Liquid distribution in a semi-industrial packed column- experimental and theory. – Scientific Works of University of Food Technology, 64, 1, 2017 (in print).

Acknowledgements

This work was financially supported by the National Science Fund at the Bulgarian Ministry of Education and Science, Contract No DN 07/14/15.12.2016

A MATHEMATICAL MODEL OF VISCOUS LIQUID MIXTURE MOTION THROUGH A VERTICAL CYLINDRICAL PIPE

Asst., MSc Sorokina Natalia,
Institute of Computer Science and Technology – Peter the Great Saint-Petersburg Polytechnic University, Russia
snv_special@inbox.ru

Abstract: In the paper a mathematical model of the non-stationary motion of a viscous liquid mixture through the vertical straight pipe of the circular cross section is proposed. During the model construction weak compressibility of the mixture is considered. The Navier-Stokes equations system is taken as a basis. Such model can be used in the description of oil motion in a vertical well.

Keywords: NON-STATIONARY HYDRODYNAMICS, LIQUID MIXTURES, WEAK COMPRESSIBILITY, VERTICAL PIPE, MATH MODELING

1. Introduction

The problem of the liquid mixtures (or emulsions, suspensions) motion is not just interesting, but also very important in some areas of the national economy, such as oil and gas industry. It is well known that during the extraction of oil it is not a “clear” product ascending from under the ground, but a mixture, consisting of oil, water and gas. In other words, we deal with the water-oil emulsion.

As emulsion move up through the tubing its properties, such as density and viscosity, are changing. Its change is connected with temperature and pressure. And it is important to know the velocity of mixture’s ascending, of course.

Further in the paper we use the term “liquid” instead of “liquid mixture” since we assume that this mixture is homogeneous – its components are distributed evenly in the main phase, they are well mixed. This is the first assumption. We have to obtain the mathematical model, describing the non-stationary motion of the weakly compressible liquid through the vertical pipe of the circular cross-section.

2. The basic equations

We take the equations of continuum mechanics as the basis [1], consider that there are no sources (or drains on the contrary) of the mass:

$$\frac{d\rho}{dt} + \rho(\vec{\nabla} \cdot \vec{v}) = 0, \quad (1)$$

$$\rho \frac{d\vec{v}}{dt} = \rho \vec{F} + \frac{\partial \vec{\tau}_x}{\partial x} + \frac{\partial \vec{\tau}_y}{\partial y} + \frac{\partial \vec{\tau}_z}{\partial z}, \quad (2)$$

$$\rho \frac{d\vec{M}}{dt} = \rho \vec{\Pi} + \vec{i} \times \vec{\tau}_x + \vec{j} \times \vec{\tau}_y + \vec{k} \times \vec{\tau}_z + \frac{\partial \vec{\pi}_x}{\partial x} + \frac{\partial \vec{\pi}_y}{\partial y} + \frac{\partial \vec{\pi}_z}{\partial z}, \quad (3)$$

$$\rho \frac{dE}{dt} = \varepsilon + \vec{\tau}_x \cdot \frac{\partial \vec{v}}{\partial x} + \vec{\tau}_y \cdot \frac{\partial \vec{v}}{\partial y} + \vec{\tau}_z \cdot \frac{\partial \vec{v}}{\partial z} + \vec{\nabla} \cdot \vec{t}. \quad (4)$$

Since we consider vertical motion, which is obviously due to the head from below, we assume that rotary motion in the liquid is absent hence we will not need the equation (3) further. As the first approximation we may assume that neither density nor pressure depends on temperature and hence energy change may be ignored. That allows us to neglect the equation (4).

3. The construction of the mathematical model

We introduce the Cartesian coordinate system and direct the axis Oz along the pipe axis. We write the system of equations (1)-(2) in projections onto the Cartesian axes:

$$\frac{\partial \rho}{\partial t} + v_x \frac{\partial \rho}{\partial x} + v_y \frac{\partial \rho}{\partial y} + v_z \frac{\partial \rho}{\partial z} + \rho \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \right) = 0, \quad (5)$$

$$\frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z} = F_x + \frac{1}{\rho} \left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \right), \quad (6)$$

$$\frac{\partial v_y}{\partial t} + v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_y}{\partial z} = F_y + \frac{1}{\rho} \left(\frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} \right), \quad (7)$$

$$\frac{\partial v_z}{\partial t} + v_x \frac{\partial v_z}{\partial x} + v_y \frac{\partial v_z}{\partial y} + v_z \frac{\partial v_z}{\partial z} = F_z + \frac{1}{\rho} \left(\frac{\partial \tau_{zx}}{\partial x} + \frac{\partial \tau_{zy}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \right). \quad (8)$$

Since it is a vertical pipe, the gravity acts on the liquid (per the elementary volume): $F_x = 0$, $F_y = 0$, $F_z = -\rho g$. Next suppose that velocity has only the vertical component, in other words $v_x = v_y = 0$. In p.2 it is said we consider that density does not depend on temperature. Let us clarify this assumption: let temperature vary with the altitude of the rise, i.e. with the change of the z coordinate, and since the density depends on temperature (also on pressure) we have an implicit density dependence on z coordinate: $\rho = \rho(T(z)) = \rho(z)$.

We write the system (5)-(8) with the assumptions described:

$$v_z \frac{\partial \rho}{\partial z} + \rho \frac{\partial v_z}{\partial z} = 0, \quad (5')$$

$$\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} = 0, \quad (6')$$

$$\frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} = 0, \quad (7')$$

$$\frac{\partial v_z}{\partial t} + v_z \frac{\partial v_z}{\partial z} = -\rho g + \frac{1}{\rho} \left(\frac{\partial \tau_{zx}}{\partial x} + \frac{\partial \tau_{zy}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \right). \quad (8')$$

In general the stress tensor components have the following form [1]:

$$\tau_{xx} = -p + \lambda \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \right) + 2\mu \frac{\partial v_x}{\partial x}, \quad (9)$$

$$\tau_{yy} = -p + \lambda \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \right) + 2\mu \frac{\partial v_y}{\partial y}, \quad (10)$$

$$\tau_{zz} = -p + \lambda \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \right) + 2\mu \frac{\partial v_z}{\partial z} \quad (11)$$

$$\tau_{xy} = \tau_{yx} = \mu \left(\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \right), \tau_{yz} = \tau_{zy} = \mu \left(\frac{\partial v_y}{\partial z} + \frac{\partial v_z}{\partial y} \right), \quad (12)$$

$$\tau_{zx} = \tau_{xz} = \mu \left(\frac{\partial v_x}{\partial z} + \frac{\partial v_z}{\partial x} \right).$$

According to the assumptions made, the stress tensor components take the following form:

$$\tau_{xx} = -p + \lambda \frac{\partial v_z}{\partial z}, \quad (9')$$

$$\tau_{yy} = -p + \lambda \frac{\partial v_z}{\partial z}, \quad (10')$$

$$\tau_{zz} = -p + [\lambda + 2\mu] \frac{\partial v_z}{\partial z} \quad (11')$$

$$\tau_{xy} = \tau_{yx} = 0, \tau_{yz} = \tau_{zy} = \mu \frac{\partial v_z}{\partial y}, \tau_{zx} = \tau_{xz} = \mu \frac{\partial v_z}{\partial x}. \quad (12')$$

Substitute these relations in the system (5')–(8'):

$$v_z \frac{\partial \rho}{\partial z} + \rho \frac{\partial v_z}{\partial z} = 0, \quad (5')$$

$$-\frac{\partial p}{\partial x} + [\lambda + \mu] \frac{\partial^2 v_z}{\partial x \partial z} = 0, \quad (6')$$

$$-\frac{\partial p}{\partial y} + [\lambda + \mu] \frac{\partial^2 v_z}{\partial y \partial z} = 0, \quad (7')$$

$$\frac{\partial v_z}{\partial t} + v_z \frac{\partial v_z}{\partial z} = -\rho g + \frac{1}{\rho} \left(\mu \frac{\partial^2 v_z}{\partial x^2} + \mu \frac{\partial^2 v_z}{\partial y^2} + \lambda \frac{\partial^2 v_z}{\partial z^2} - \frac{\partial p}{\partial z} \right). \quad (8')$$

Let us turn to the cylindrical coordinates in the system (5')–(8'), assuming in advance the cylindrical symmetry of the flow:

$$v_z \frac{\partial \rho}{\partial z} + \rho \frac{\partial v_z}{\partial z} = 0, \quad (5')$$

$$[\lambda + \mu] \cos \varphi \frac{\partial^2 v_z}{\partial r \partial z} - \cos \varphi \frac{\partial p}{\partial r} = 0, \quad (6')$$

$$[\lambda + \mu] \sin \varphi \frac{\partial^2 v_z}{\partial r \partial z} - \sin \varphi \frac{\partial p}{\partial r} = 0, \quad (7')$$

$$\frac{\partial v_z}{\partial t} + v_z \frac{\partial v_z}{\partial z} = -\rho g + \frac{1}{\rho} \left(\mu \left[\frac{\partial^2 v_z}{\partial r^2} + \frac{1}{r} \frac{\partial v_z}{\partial r} \right] + \lambda \frac{\partial^2 v_z}{\partial z^2} - \frac{\partial p}{\partial z} \right). \quad (8')$$

Next we add two equations (6') and (7'):

$$[\lambda + \mu] [\cos \varphi + \sin \varphi] \left(\frac{\partial^2 v_z}{\partial r \partial z} - \frac{\partial p}{\partial r} \right) = 0.$$

Since sum of bulk and dynamic viscosity coefficients cannot be zero, sum of sine and cosine of the same angle cannot be zero, it follows that

$$\frac{\partial^2 v_z}{\partial r \partial z} - \frac{\partial p}{\partial r} = 0,$$

or

$$\frac{\partial^2 v_z}{\partial r \partial z} = \frac{\partial p}{\partial r}. \quad (13)$$

Thus the final system of equations has the following form (we omit the z index since we assume that there is only one velocity component):

$$v \frac{\partial \rho}{\partial z} + \rho \frac{\partial v}{\partial z} = 0, \quad (5')$$

$$\frac{\partial^2 v}{\partial r \partial z} = \frac{\partial p}{\partial r}, \quad (13)$$

$$\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial z} = -\rho g + \frac{1}{\rho} \left(\mu \left[\frac{\partial^2 v}{\partial r^2} + \frac{1}{r} \frac{\partial v}{\partial r} \right] + \lambda \frac{\partial^2 v}{\partial z^2} - \frac{\partial p}{\partial z} \right). \quad (8')$$

Three equations contain three unknown functions: density $\rho(z)$, pressure $p(z)$ and velocity $v(r, z, t)$.

4. The formulation of the corresponding problem and its correctness

As noted earlier, the problem of studying the motion of a viscous liquid (liquid mixture) through the vertical pipe arises in the

field of oil products extraction. It is necessary to predict the pressure, viscosity and velocity of the mixture that rises from the depth along the pipe, to understand whether, for example, pressure changes are so critical that it will lead to partial equipment destruction (the same pipe).

For the mathematical formalization of the corresponding problem, it is necessary to set the initial pressure at the pipe inlet and pipe outlet (at the pipe outlet it is possibly constant), initial velocity distribution over the cross-section and initial density of the liquid. In time, or, in the first approximation, during the ascending along the change in pressure the liquid density changes, since the saturation of the mixture with gas increases [4,5].

In solving partial differential equations (systems of equations), the study of the correctness of the corresponding initial-boundary value problems for equations being solved is especially important. For quasilinear partial differential equations of the second order this analysis is not simple. For the system of equations (5'), (13), (8'), such a study was carried out by O.A. Ladyzhenskaya [2]. The results are positive.

5. The solution method

For the initial-boundary value problem, the system of equations obtained in p.3 can be solved by a numerical method – the variable direction method [3]. According to this method, the previously obtained partial differential equations are replaced by difference relations with intermediate computation of functions on the $k + 0.5$ -th time layer: A similar solution has already been applied in [4].

6. Conclusion

In this paper, the construction of a mathematical model describing the nonstationary motion of a viscous compressible mixture over a long vertical rectilinear tube of circular cross-section is considered. Such a model can be used to solve the problem of the movement of oil along a vertical well. A numerical method for solving the corresponding initial-boundary value problem is proposed.

7. References

- [1] Vallander, S.V. Lectures on fluid dynamics. – L.: Izd-vo Leningr. un-ta, 1973, 296 p. (in Russian)
- [2] Ladyzhenskaya, O. A. On the unique solvability in the large of the three-dimensional Cauchy problem for the Navier-Stokes equations in the presence of axial symmetry (in Russian), Zapiski Nauchnikh Seminarov LOMI, 1968, v. 7, p. 155-177
- [3] Filatov, E. Y., Yasinskiy, F. N. Mathematical modeling of liquid and gas flows: Tutorial / State Educational Institution of Higher Professional education "Ivanovo Power Engineering Institute of V. I. Lenin". – Ivanovo, 2007 (in Russian)
- [4] Firsov A., Sorokina N. Mathematical modeling of non-stationary flows of liquid homogeneous viscous mixtures by pipelines // Mathematical modeling. – 2017. – Issue 1/2017. – P.18-22
- [5] Islamov M.K. Borehole oil extraction [Electronic resource]: Theoretical basis for lifting fluid and gas from a well URL: http://doidpo.rusoil.net/storage/Downhole%20oil%20production%20Islamov%29/to/to4_1.html (access date: 21.11.17) (in Russian)
- [6] Everything about oil [Electronic resource]: Oil extraction. Methods of operation of wells. URL: <http://vseonefti.ru/upstream/sposoby-dobychi.html> (access date: 21.11.17) (in Russian)

COMPUTER SYSTEM FOR PREDICTING THE STRUCTURE AND PROPERTIES OF CAST METAL PRODUCTS

Ass. Prof., Dr. Eng. Donii O., Ass. Prof., Dr. Eng. Kulinich A., Ass. Prof., Dr. Eng. Khristenko V.
National Technical University of Ukraine "Kyiv Polytechnic Institute named after Igor Sikorsky" - Kyiv, Ukraine
Email: dosha@iff.kpi.ua

Abstract: The basic principles of functioning of subsystems of the information-technological complex, which is intended for the forecast of structure and properties of the cast metal, are presented. The basis of subsystems are mathematical and simulation models of crystallization. The subsystem of thermal analysis is based on mathematical models, which were developed within the framework of the dynamic theory of metallic castings. The subsystem of modeling of crystallization is based on a combination of mathematical models of heat conduction and diffusion with cellular automata. The model makes it possible to investigate in computational experiment the effect of various cooling conditions on the process of formation of the structure during crystallization. The results of computer experiment are shown.

KEYWORDS: COMPUTER THERMAL ANALYSIS, SIMULATION MODELING, CRYSTALLIZATION, STRUCTURE OF METALS AND ALLOYS, COMPUTER MODELING, CELLULAR AUTOMATON

1. Introduction

One of the factors to solve the problem of improving the quality of castings and increasing the efficiency of foundry production is the availability of methods for the on-line monitoring of the melting process and evaluation of the melt's state immediately before casting. Although the process of forming the quality of metal products is complex and multistage, crystallization plays a special role in it since it is at this stage the "primary" structure of solid metal is formed, which significantly influences the formation of the properties, which the final product must have. That is, it is necessary to be able to on-line check of the melt's state and control the crystallization process during the technological process of smelting. As one of the variants of realization of this task it is possible to use information-technological complex consisting of subsystems of computer thermal analysis [1] and of simulation modeling of metals' and alloys' crystallization [2]. Thermal analysis provides information on thermal effects during hardening of sample, which reflect the processes of formation of the cast metal's structure. This makes it possible to analyze the kinetics of the crystallization process using data of the cooling curve and to predict the service properties of metals and alloys in the solid state. Simulation modeling makes it possible in the mode of computer experiment to optimize known and develop new technological modes for creating foundry products, which significantly reduces time of development and material costs, gives an opportunity to obtain important scientific information about the process of crystallization of metals and alloys under both equilibrium and nonequilibrium conditions (even those ones, which is difficult or impossible to obtain under in laboratory conditions). Simulation modeling makes it possible in the mode of computer experiment to optimize known and develop new technological modes for creating foundry products, which significantly reduces time of development and material costs, gives an opportunity to obtain important scientific information about the process of crystallization of metals and alloys under both equilibrium and nonequilibrium conditions.

2. Preconditions and means for resolving the problem

The thermal analysis subsystem should record the change of the temperature of metallic material, which is in the process of crystallization (the cooling curve). Using the data of the cooling curve with the help of mathematical modeling it is possible to single out information on the dynamics of the crystallization process, which helps to predict the properties of metals or alloys in the solid state. Mathematical models in this case should be simple, since the calculations based on them must be performed in the computer for the minimum possible time [3]. Similar models are proposed in the framework of the dynamic theory of hardening of metallic castings [4]. Based on these models, a technique for computer thermal analysis is proposed, which simulates differential thermal analysis using the hardware of simple thermal analysis. The application of this technique significantly increases the sensitivity of the method, as well as the reliability of the forecast of the structure and properties of the metal in the solid state.

In the process of developing of a subsystem of simulation modeling of the formation of the structure of metallic materials during their crystallization, problems arise due to the complexity of the mathematical formulation of the problem. At the same time, studies of cellular automata have shown the principal possibility of their use for modeling of similar processes [5]. However, the rules for cellular automata' operation of are usually given without connection with real physical processes. In this paper we propose a simulation model of crystallization, which is based on combination of mathematical models of heat conduction and diffusion with cellular automata. At that, the external cooling conditions and composition of the liquid metal or melt at a certain point determine the possible state (liquid or solid) of the corresponding cell of the cellular automaton.

3. Structure and capabilities of the models

3.1. The subsystem of computer thermal analysis

Mathematical difficulties which arise while creating mathematical models of crystallization can be significantly reduced if we consider the case of solidification of a body whose temperature gradient across its volume can be neglected. In the method of thermal analysis, which is used in this work, portions of metal or metal alloys which have small dimensions and cylindrical shape with a diameter of 20 ... 40 mm are examined. Since metallic materials are good conductors of heat, in this case it is possible to proceed to an analysis of the heat balance equation for the whole sample as a whole [4]. Then the heat balance equation is represented as:

$$\frac{dQ}{dt} = \frac{dQ_c}{dt} + \frac{dQ_L}{dt}, \quad (1)$$

where $\frac{dQ}{dt}$ - the change in the amount of heat in the sample due to

its release into the environment; $\frac{dQ_L}{dt}$ - change in the amount of

heat, which is released as a result of formation of a solid phase;

$\frac{dQ_c}{dt}$ - change in the amount of heat in the sample due to changes

of the material's temperature.

Substituting the known relations in (1):

$$dQ_c = -cmd(t), \quad (2)$$

$$\frac{dQ}{dt} = fS[T(t) - T_{cp}] + \sigma \varepsilon S[T^4(t) - T_{cp}^4], \quad (3)$$

we obtain the differential equation in the form:

$$\frac{dT(t)}{dt} + k_1[T(t) - T_{cp}] + k_2[T^4(t) - T_{cp}^4] = Z(t), \quad (4)$$

$$\text{where } Z(t) = \begin{cases} 0, & \text{при } t \leq t_{kp}, t \geq t_{ms} \\ \frac{L}{c} \frac{m(t)}{m_0}, & \text{при } t_{kp} \leq t \leq t_{ms} \end{cases} \quad (5)$$

$$V(t) = \frac{m(t)}{m_0}, \quad (6)$$

$$k_1 = \frac{fS}{cm_0}, \quad (7)$$

$$k_2 = \frac{\sigma \varepsilon S}{cm_0}, \quad (8)$$

where $T(t)$, T_{cp} - are the temperatures of the metal (of cooling curve) and of the environment; t - is the total time of the process; t_{kp} - is the time of onset of crystallization; t_{me} - time of the end of crystallization; c , L , m_0 - are, respectively, specific heat, specific latent heat of crystallization and portion's mass of the material that is being investigated; $m(t)$ - is the mass of the solidified part of the sample to the instant t ; ε - is the degree of blackness of the cooling surface; $\sigma = 5,56 \cdot 10^{-8} \text{ Дж/(м}^2 \cdot \text{К}^4)$ - is the Stefan-Boltzmann constant.

Equation (4) simulates the technique of differential thermal analysis, which has a high sensitivity of the beginning and end of phase transformations. During the experiment, the cooling curve $T(t)$ is fixed in the computer memory. Then, its fourth degree and derivative are calculated. Knowing the values of the coefficients k_1 , k_2 , we can calculate the right-hand side of $Z(t)$ equation (3). Before the beginning of crystallization and after its termination, the value of Z is zero. During crystallization, heat is released and the balance is disrupted. These changes at the points t_{kp} and t_{me} are easily recorded in the experiment.

To determine the values of the coefficients k_1 and k_2 , the initial and final sections of the cooling curve are used, where there is no release of crystallization heat and the right-hand side of equation (4) is zero. These sections of the cooling curve are linearized by dividing of both parts (4) by $[T(t) - T_{cp}]$ and introducing of new variables:

$$x = \frac{T^4(t) - T_{cp}^4}{T(t) - T_{cp}}, \quad (9)$$

$$y = -\frac{T'(t)}{T(t) - T_{cp}}. \quad (10)$$

Then equation (4) in these areas becomes the equation of a straight line:

$$y = k_1 + k_2 x. \quad (11)$$

The values of the coefficients are determined by the method of least squares [6].

Thus, this technique of computer thermal analysis uses the hardware part of simple thermal analysis and simulates differential thermal analysis. Its use in the subsystem of the computer thermal analysis makes it possible to analyze the kinetics of the crystallization process using the data of the cooling curve and to predict the service properties of metals in the solid state.

3.2. The subsystem of simulation modeling

The two-dimensional heat equation is used in the development of the subsystem of simulation modeling of formation of the structure of metallic materials during their crystallization. It assumes that cooling of the body comes from all four sides of the plane, and thermophysical characteristics of the melt (specific heat, density and thermal conductivity) do not depend on temperature (ie, c , ρ , λ = const):

$$\frac{\partial T(x, y, t)}{\partial t} = a \left(\frac{\partial^2 T(x, y, t)}{\partial x^2} + \frac{\partial^2 T(x, y, t)}{\partial y^2} \right) \pm \frac{L}{c} \frac{\partial \varepsilon(x, y, t)}{\partial t}, \quad (12)$$

$$T(x, y, 0) = T_0 = \text{const}, \quad (13)$$

$$\frac{\partial T(0, y, t)}{\partial x} = -\alpha_1 [T(0, y, t) - T_0], \quad (14)$$

$$\frac{\partial T(x_0, y, t)}{\partial x} = -\alpha_2 [T(x_0, y, t) - T_0], \quad (15)$$

$$\frac{\partial T(x, 0, t)}{\partial y} = -\alpha_3 [T(x, 0, t) - T_0], \quad (16)$$

$$\frac{\partial T(x, y_0, t)}{\partial y} = -\alpha_4 [T(x, y_0, t) - T_0], \quad (17)$$

where $a = \frac{\lambda}{c\rho}$ - is the coefficient of thermal diffusivity; $\varepsilon(x, y, t)$ - is

the fraction of the solid phase in some elementary volume; T_0 - is the initial temperature; L - is the specific latent heat of crystallization; α_1 , α_2 , α_3 , α_4 - heat transfer coefficients from four sides; x_0 , y_0 - are the dimensions of the system. The last term in the heat equation.

The last term in the heat equation (12) takes into account the release (or absorption) of heat during the phase transformation. Since a cellular automaton is used in the simulation model of crystallization, it is convenient to solve this problem numerically. This solution is realized by the splitting method using an implicit numerical scheme.

Taking into account the need to enter the system time in the model, the order of calculations is organized as follows. First and foremost, the heat conduction problem is solved numerically, in which the time step determines the system time of the entire model. At that, one step of the system time is the total time of observation of the diffusion problem. Therefore, the calculation of this task is carried out anew at each step of the system time. At that, the initial condition changes each time: the previous solution becomes a new initial condition. The boundary conditions assume the absence of exchange of matters at the boundaries of the system:

$$\frac{\partial K(x, y, t)}{\partial t} = D \left(\frac{\partial^2 K(x, y, t)}{\partial x^2} + \frac{\partial^2 K(x, y, t)}{\partial y^2} \right), \quad (18)$$

$$K(x, y, 0) = K_0(x, y), \quad (19)$$

$$\frac{\partial K(0, y, t)}{\partial x} = 0, \quad (20)$$

$$\frac{\partial K(x_0, y, t)}{\partial x} = 0, \quad (21)$$

$$\frac{\partial K(x, 0, t)}{\partial y} = 0, \quad (22)$$

$$\frac{\partial K(x, y_0, t)}{\partial y} = 0, \quad (23)$$

where $K(x, y, t)$ - is concentration of the second component in the melt; $K_0(x, y)$ - is an initial concentration, which is updated at each step of the system time; D - is the diffusion coefficient of the second component of the alloy in the melt. The solution of this problem is completely analogous to the solution of the thermal problem.

The temperature and concentration of the second component at each point of melt determine the size of the local supercooling, which is calculated as the difference of the liquidus temperature for this point and its temperature at a given time. Subcooling in the liquid state is the main driving force of crystallization. In its presence, there are conditions for formation of a crystal or growth of an already existing embryo. To calculate the presence and magnitude of supercooling, the linearization of the liquidus lines and of the solidus of the double-alloy state diagram with the eutectic is used.

Thus, in the subsystem of simulation modeling, mathematical models of heat conduction and diffusion are organized in such a way that it is possible to simulate various conditions of cooling which take place during crystallization in the technological processes of foundry. The simulation model itself has the possibility of changing the cooling conditions (reducing or increasing the intensity of the heat removal) directly in the course of the computer experiment.

4. Results and discussion

The basis for predicting of the mechanical properties of the alloys of the AL-Si and Al-Si-Mg systems in the cast state is that the temporary tear resistance σ_e and relative elongation δ are mainly determined by the chemical composition of alloys' main alloying components (Si, Mg) and impurities, which significantly affect the mechanical properties of these alloys (for example, Fe). In addition,

inherited metal's properties and technology's factors that are difficult to control (for example, overheating or modifying) can also change the average level of mechanical properties. The total effect of these factors is manifested in the thermogram in the form of a change in the values of recalcence during the formation of the α -phase and the eutectic. As shown in [3], these parameters, in particular eutectic recalcence, correlate with the level of mechanical properties. Therefore, it is advisable to introduce its value as an additional parameter into equation of forecasting of mechanical properties. To create appropriate regression equations, experiments were performed in which content of the silicon for Al-Si and Al-Si-Mg alloys varied from 6.1% to 11.3% and of magnesium - in the range from 0.15% to 0.40%. Equations are obtained for the alloy of the Al-Si system, which bind the temporary tear resistance and relative elongation with the calculated content of silicon, iron, and with the value of eutectic recalcence. They have the following form:

$$\sigma_s = 14,37145 + 0,31076 \cdot Si - 13,1125 \cdot Fe - 9,3304 \cdot Fe^2 + 0,2431 \cdot \Delta T_{sp}, \quad (24)$$

$$\delta = 4,4195 - 0,16663 \cdot Si - 1,7786 \cdot Fe - 1,06714 \cdot Fe^2 + 0,0283 \cdot \Delta T_{sp}, \quad (25)$$

а для сплава системы Al-Si-Mg:

$$\sigma_s = 51,01231 + 4,13723 \cdot Si + 8,05964 \cdot Mg - 4,6346 \cdot Fe + 0,01782 \cdot \Delta T_{sp}, \quad (26)$$

$$\delta = -2,1175 - 1,3332 \cdot Si - 0,2143 \cdot Mg - 5,60762 \cdot Fe + 0,0171 \cdot \Delta T_{sp}, \quad (27)$$

where ΔT_{sp} - the value of the recalcence of temperature, determined by the cooling curve in the region of formation of the eutectic. Composition of alloys is also determined by the cooling curve by means of the method, which is described in [3]. Fisher criterion was used to prove the adequacy of the models, and the error in forecasting of the properties was 5 ... 7%. When testing the subsystem of computer thermal analysis under industrial conditions, the equations described above showed the convergence of results and the accuracy of the prediction of properties at the level of standard methods of mechanical testing.

The use of cellular automata greatly simplifies mathematical calculations while usage of the model and gives the principal possibility of modeling of the emerging polycrystalline structure of metallic materials. The influence of the external cooling conditions of the system under study on the functioning of the cellular automaton makes it possible to establish technological methods for

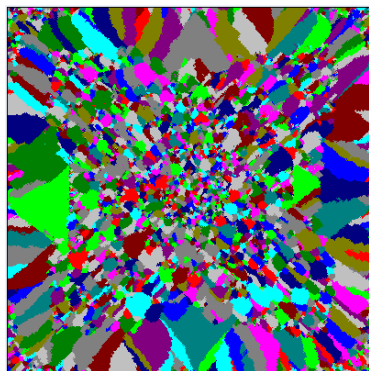


Fig. 1. Macrostructure of pure aluminum, which is simulated at speed of cooling 5 deg/s

obtaining various structures of solid metal. Model structures were obtained as a result of the computer experiment of homogeneous crystallization of aluminum with usage of various cooling speed during the process.

With equal speed of heat removal from all sides and a cooling rate of 5 deg/s, a diverse granular structure of pure aluminum is formed (Fig. 1). There are small grains in the center, and on the sides grains'

sizes are much larger. It can be also observed that a solid metal's structure is interrelated with the shape of the temperature's field inside the system. Figure 2 shows the structure of aluminum, which

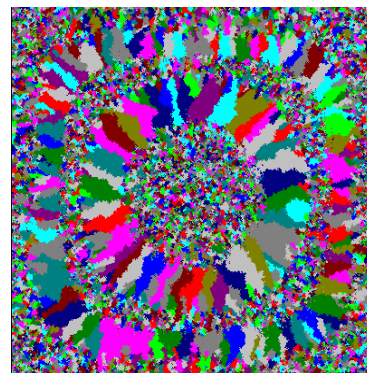


Fig. 2. Macrostructure of pure aluminum, simulated by an alternate change in the coefficients of heat transfer in the process of crystallization

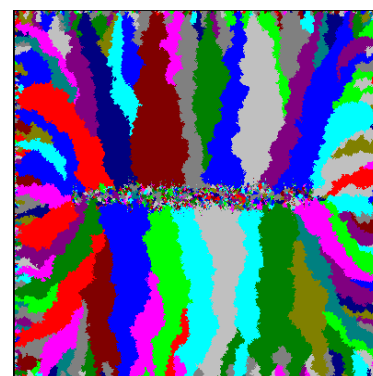


Fig. 3. Macrostructure of pure aluminum, simulated with asymmetric variation of heat transfer coefficients

was obtained by repeatedly changing intensity of heat removal. At first, fine grains were formed at the boundaries of the system in conditions of high cooling rate. Then the intensity of heat removal from all sides was reduced symmetrically and the size of the growing grains increased. After some time, the cooling rate was increased, then reduced and then increased again. As a result, the final structure consists of several alternating areas with different shapes and different average sizes of grains (Fig. 2). Complex aluminum structure has been obtained in which grains of different shapes, sizes, and orientations are observed (Fig. 3) as a result of varying of the cooling rate by setting asymmetrical coefficients of heat removal from different sides and by varying of their magnitude. It can be assumed that in this case the properties of the real metal will have anisotropy. Such regimes of crystallization are not easy to be realized in practice, but these experiments demonstrate the capabilities of this modeling subsystem.

5. Conclusion

1. Usage of mathematical models of solidification of a small portion of metal allows to increase the sensitivity of thermal analysis to the level of differential thermal analysis due to calculating of the sample's heat balance before, after and during crystallization.
2. The resulting regression equations allow to predict the level of breaking point and relative elongation of alloys of Al-Si and Al-Si-Mg systems using data from the cooling curve of the thermal analysis with an error of 5 ... 7%.
3. Simulation model of crystallization makes it possible to visualize the process of formation of the macro structure of metals under different conditions of crystallization, that makes it possible, within the framework of a computer experiment, to develop techniques for management of this process to obtain the necessary properties of cast products.

4. Combination of the subsystem of simulation modeling of crystallization and subsystem of computer thermal analysis as part of the informational and technological complex significantly expands possibilities of controlling the cast products' quality and allows to obtain information by engineers-technologists both in applied and in theoretical aspects.

6. Literature

1. Donii O. System of control and management of the quality of foundry melts on the basis of computer thermal analysis. Acta Universitatis Pontica Euxinus. Dnipropetrovsk, Varna, Volume III, 2011, P. 84 - 87. (Ukrainian)

2. Donii O. Modeling of metal crystallization by means of cellular automation Materials science. Non-equilibric phase transformations, 4, 2017, P. 150 - 153.

3. Bialik O. Donii O., Golub L. Forecast of properties of metals and alloys by the method of computer thermal analysis. Preprint, Kyiv, "Politechnika". (Ukrainian)

4. Bialik O., Mentkovskiy Yu. Questions of the dynamic theory of hardening of metal castings. Kiev, Higher school, 1983. (Russian)

5. Hayes B. The cellular automaton creates a model of the world and the world around itself. In the world of science. N5, 1984, p. 97 - 104. (Russian)

6. Lvovskyi E. Statistical methods of constructing of empirical formulas. M, Higher school, 1988. (Russian)

DECISION OF OPTIMIZATION PROBLEMS USING SYMMETRIC ALGORITHM OF HEAVY BALL METHOD

Kharlamova Y.N.
National Mining University, Dnipro, Ukraine
E-mail: harlamyshka@gmail.com

Abstract: The algorithm of the heavy ball method, based on the principle of symmetry, to find a global extremum is described. The computer simulation of the method for the three test functions (Ackley, Griewank and Schwefel) is carried out. The results of the study of the efficiency of this algorithm are given. The results of mathematical modeling in the graphs, describing the process of convergence of representative points to the global optimum point of test functions, are shown. Conclusions about the efficacy of the described algorithm applied to optimization problems are drawn.

KEYWORDS: HEAVY BALL METHOD, ENERGY INTERACTION BETWEEN THE TWO BALLS, EXTREMUM SEEKING PROCESS, CONCEPT OF SYMMETRY

Y.

1. Introduction

One of the main factors that must be considered in solving the problems of synthesis of modern adaptive identification systems and information measuring systems is the inertia of the control object and measuring equipment. The creators of these systems use various optimization methods to ensure high efficiency of taken decisions.

In most cases, the seeking global extremum of multiextremal objective functions is carried out dynamically using the heavy ball method. But a moving heavy ball can have both a lack of kinetic energy and an excess of it. In the first case, it can stop at the one of the local extremes, before reaching the global extremum, and in the second case - to jump over it.

In the current situation, it is actual to organize the boosting of additional kinetic energy of the ball moving to the global extremum or to remove its excess.

2. Analysis of the literature sources

Today, both global optimization algorithms for solving a separate class of problems [1] and for more universal ones have been developed. When considering dynamic optimization problems, the relaxation method [2,3] is often applied, the realization of which is carried out by means of nonstationary processes that are described by vector differential equations of the form

$$(1) m \cdot x^{(2)}(t) + r \cdot x^{(1)}(t) + \text{grad} f(x) = 0, \quad m > 0, \quad r > 0;$$

$$(2) \frac{dx}{dt} + k \text{grad} f(x) = 0, \quad k > 0.$$

These processes to solve the task are eventually established.

The equation (1) describes the *heavy ball method*, which (with an appropriate choice of the parameters m and r) is referred to methods of seeking for a global extremum. The relaxation method, realized according to equation (2), is called the *steepest gradient descent method*, it is usually referred to methods of seeking for a local extremum of the function.

It is known that surface elongation of the objective function along one of the directions and its complex relief sharply worsens the effectiveness of these methods. The heavy ball method and the steepest gradient descent method in solving seeking global extremum problems, with an increase of the oscillations amplitude do not give a positive result, and the process of motion of the representing point stops at the first local extremum.

The purpose of the article is to construct algorithms for seeking for a global extremum of functions based on the principle of symmetry of the interaction of two heavy balls and to justify the advantage of this algorithm in seeking for a global extremum of the multiextremal function in comparison with other relaxation algorithms.

3. Results and discussion

The problem of seeking for the minimum of a multiextremal function can be solved by using the concept of symmetry, which has proven itself in such one-dimensional optimization methods such as methods of dichotomy, Fibonacci and golden section. In these methods, two *representative* points move symmetrically to the extremum of the function, significantly reducing the interval of uncertainty (localization).

Let us consider multidimensional methods improving process of function extremum seeking by applying the concept of symmetry [4,5].

Let us represent the expression of a downward-convex function $f(x)$ (x is a vector argument), which extremum is sought, in the form

$$(3) f(x) = 0.5 \left((x-x)^T Q(x-x) + f(x) + f(x) \right),$$

where Q is a positive definite symmetric matrix.

Then, replacing one of the vectors x with the vector y and the other with the vector z in the expression (3), we obtain an auxiliary function

$$(4) F(y, z) = 0.5 \left[(y-z)^T Q(y-z) + f(y) + f(z) \right],$$

the extremum of which will take place under the condition that $y=z=x^*$, where x^* is the value of the vector argument at which the function $f(x)$ takes an extreme value.

The motion to a minimum of the auxiliary function $F(y, z)$ is ensured as a result of a simultaneous coherent change of vector arguments y and z by any of the known extremum seeking algorithms.

The algorithm (1) of a heavy ball method [6,7] when working with an auxiliary function $F(y, z)$ will be such as

$$(5) \begin{aligned} m \frac{d^2 y}{dt^2} + r \frac{dy}{dt} + \frac{\partial F(y, z)}{\partial y} &= 0, \\ m \frac{d^2 z}{dt^2} + r \frac{dz}{dt} + \frac{\partial F(y, z)}{\partial z} &= 0. \end{aligned}$$

It should be noted that for the extremum seeking of the auxiliary function (5), both continuous and discrete algorithms of several converging points can be used. This allows them to overcome local extremes.

Let us consider the efficiency of the heavy ball method, based on the principle of symmetry, on the example of three standard test functions: Ackley, Griewank and Schwefel [8].

The Ackley function (Fig. 1, a) has many local extremums near the global optimum. On the interval $[-7; 3]$, the function takes a minimum value at the point 0, where $x=0$ and corresponds to the following description

$$(6) f(x) = 20 + e - 20 \cdot \exp(-0.2 \sqrt{\frac{1}{n} \sum_{i=1}^n x_i^2}) - \exp(\frac{1}{n} \sum_{i=1}^n \cos(2\pi x_i)).$$

Then the auxiliary symmetric function $F(y, z)$ according to the equation (4) for the Ackley function (6) will have the following form:

$$(7) F(y, z) = 0.5(2(20 + e) - 20 \exp(-0.2 y^2) - \exp(\cos(2\pi y))) - 20 \exp(-0.2 z^2) - \exp(\cos(2\pi z)) + 0.5q(y - z)^2,$$

and the corresponding algorithm (5) for the function (7)

$$(8) \begin{cases} y_1'(t) = y_2, \\ y_2'(t) = -\frac{r}{m} y_2 - \frac{1}{m} \left[q(y_1 - z_1) + 2y_1 \sqrt{y_1^2} \exp(-0.2 \sqrt{y_1^2}) + \pi \sin(2\pi y_1) \exp(\cos(2\pi y_1)) \right], \\ z_1'(t) = z_2, \\ z_2'(t) = -\frac{r}{m} z_2 - \frac{1}{m} \left[q(z_1 - y_1) + 2z_1 \sqrt{z_1^2} \exp(-0.2 \sqrt{z_1^2}) + \pi \sin(2\pi z_1) \exp(\cos(2\pi z_1)) \right]. \end{cases}$$

where $y_1 = y, \quad z_1 = z$.

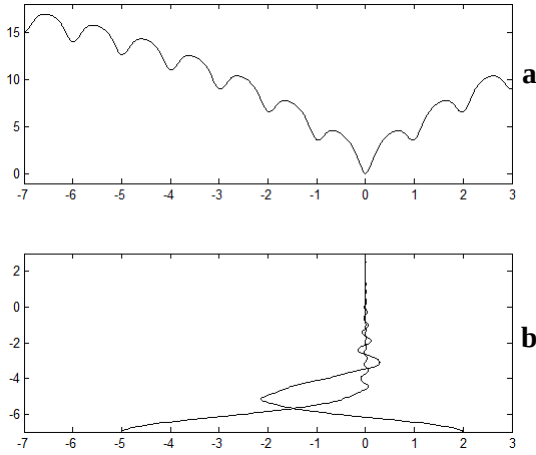


Fig.1. Graphs illustrating the process of the global extremum seeking of a function with use of the concept of symmetry: a - the type of the Ackley test function; b - solution of the system (8)

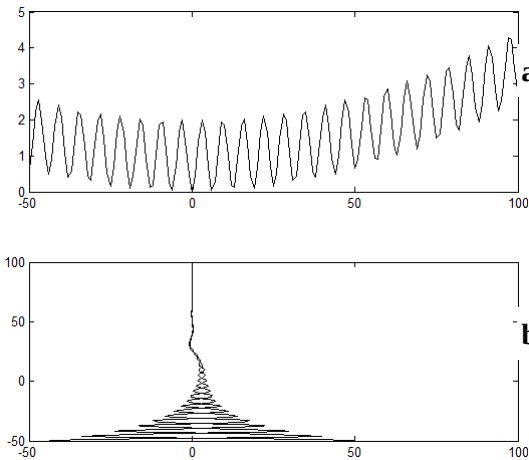


Fig.2. Graphs illustrating the process of the global extremum seeking of a function with the use of the concept of symmetry: a - the type of the Griewank test function; b - solution of the system (11)

For the solution of the system (8) initial conditions were set: $y_1(0) = -5, z_1(0) = 2$ and the following parameters were chosen: a mass of a heavy ball $m = 1.5$, damping coefficient $r = 2$ and $q = 2$. Fig. 1(b) shows the result of the solution of the system (8), which describes the process of convergence of the *representative* points to the point of the global optimum ($x^* = 0$). The following values are obtained: $y_1 = 0.000002$ and $z_1 = -0.001472$. The solution of the problem (6) with the usual heavy ball method according to the expression (1), with constant values of the parameters m and r , gave the following results: $x = -4.9862$ (from the initial point $x(0) = -5$) and $x = 1.9745$ (from the point $x(0) = 2$).

There are many local minimums in the *Griewank* function (Fig. 2, a). On the interval $[-50; 100]$, the function takes a minimum value at the point 0, where $x = 0$ and has such description

$$(9) f(x) = 1 + \sum_{i=1}^n \frac{x_i^2}{4000} - \prod_{i=1}^n \cos\left(\frac{x_i}{\sqrt{i}}\right).$$

Then the auxiliary symmetric function $F(y, z)$ for the *Griewank* function (9) is written so

$$(10) F(y, z) = 0.5(2 + \frac{y^2}{4000} - \cos(y) + \frac{z^2}{4000} - \cos(z)) + 0.5q(y - z)^2$$

and the corresponding algorithm (5) for the function (10)

$$(11) \begin{cases} y_1'(t) = y_2; \\ y_2'(t) = -\frac{r}{m} y_2 - \frac{1}{m} \left[q(y_1 - z_1) + \frac{y_1}{4000} + 0.5 \sin(y_1) \right], \\ z_1'(t) = z_2; \\ z_2'(t) = -\frac{r}{m} z_2 - \frac{1}{m} \left[q(z_1 - y_1) + \frac{z_1}{4000} + 0.5 \sin(z_1) \right]. \end{cases}$$

For the solution of the system (11) initial conditions were set: $y_1(0) = -47, z_1(0) = 53$ and the following parameters were chosen: a mass of a heavy ball $m = 7$, damping coefficient $r = 1$ and $q = 2$. Fig. 2(b) shows the result of the solution of the system (11), which describes the process of convergence of the *representative* points to the point of the global optimum ($x^* = 0$). The calculated values were: $y_1 = -0.000254$ and $z_1 = -0.000862$. The solution of the problem (9) with the usual heavy ball method according to the expression (1) gave the following results: $x = -43.9603$ (from the initial point $x(0) = -47$) and $x = 50.2403$ (from the point $x(0) = 53$).

The *Schwefel* function (Fig. 3(a)) as well as the two above-mentioned functions, has a local minimums near global optimum. On the interval $[-500; 500]$, the function takes a minimum value at the point 0, where $x = 420$ and corresponds to the following description

$$(12) f(x) = 418.9829 \cdot n + \sum_{i=1}^n (-x_i \cdot \sin(\sqrt{|x_i|})).$$

For the *Schwefel* function (12), the auxiliary symmetric function $F(y, z)$ will be

$$(13) F(y, z) = 0.5(2 \cdot 418.9829 - y \sin(\sqrt{|y|}) - z \sin(\sqrt{|z|})) + 0.5q(y - z)^2,$$

and the corresponding algorithm (5) for the function (13)

$$(14) \begin{cases} y_1'(t) = y_2; \\ y_2'(t) = -\frac{r}{m}y_2 - \frac{1}{m} \left[\frac{q(y_1 - z_1) - 0.5\sin(\sqrt{|y_1|}) - y_1 \cos(\sqrt{|y_1|}) \cdot \text{sign}(y_1)}{4\sqrt{|y_1|}} \right]; \\ z_1'(t) = z_2; \\ z_2'(t) = -\frac{r}{m}z_2 - \frac{1}{m} \left[\frac{q(z_1 - y_1) - 0.5\sin(\sqrt{|z_1|}) - z_1 \cos(\sqrt{|z_1|}) \cdot \text{sign}(z_1)}{4\sqrt{|z_1|}} \right]. \end{cases}$$

For the solution of the system (14) initial conditions were set: $y_1(0) = -200, z_1(0) = 480$ and the following parameters were chosen: a mass of a heavy ball $m = 57.8$, damping coefficient $r = 0.67$ and $q = 2$. Fig. 3(b) shows the result of the solution of the system (14), which describes the process of convergence of the *representative* points to the point of the global optimum ($x^* = 420$). The following values are obtained: $y_1 = 420.0194$ and $z_1 = 420.0862$. The solution of the given problem (12) by the heavy ball method according to the equation (1) from the initial point $x(0) = -4.5$ did not give a positive result, the representing point completed its motion at $x = -124.8345$, from the point $x(0) = 3.75$ the global optimum point is found with a low accuracy $x = 420.8741$.

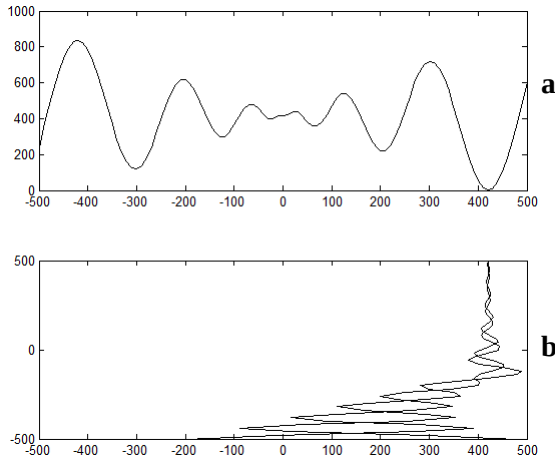


Fig.3. Graphs illustrating the process of the global extremum seeking of a function with the use of the concept of symmetry: a - the type of the Schwefel test function; b - solution of the system (14)

Let us analyze the work of the heavy ball method by comparing it with the method of coordinate descent and the gradient method with a constant step, applying the concept of symmetry to them. The algorithm of the steepest gradient descent method of when working with $F(y, z)$ is:

$$(15) \begin{cases} \frac{dy}{dt} = -kQ(y - z) - 0.5k \text{grad } f(y), & y(0) = y_0 \\ \frac{dz}{dt} = -kQ(z - y) - 0.5k \text{grad } f(z), & z(0) = z_0, \end{cases} \quad y_0 \neq z_0.$$

In contrast to the differential equation (1), which may be represented as a system of two first order differential equations and which describes the motion of one representative point, the algorithm (15) describes the energy interaction of two representative points. These points form a single system.

Let us study the work of the principle of the concept of symmetry by applying it to a function:

$$(16) f(x) = k \cdot (x - a)^2 - c \cdot \cos(2\pi x) + b,$$

the graph of which is shown in Fig.4(a). It can be seen from Fig. 4(a) that the function under consideration has local extremums, which are located near the global extremum, which is at the point with the coordinate $x = 4$.

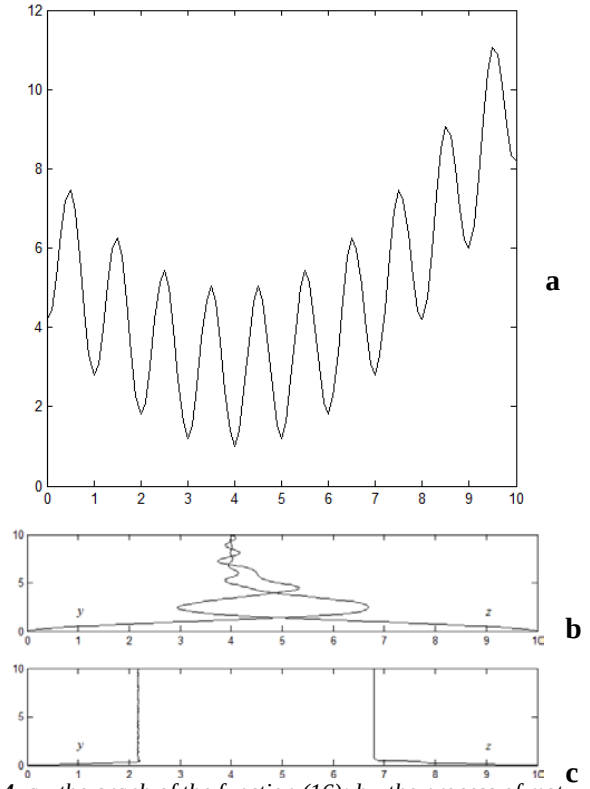


Fig. 4. a - the graph of the function (16); b - the process of motion of the representative points to the global extremum according to the algorithm of the heavy ball method, c - according to the gradient method.

Using equation (4), for the function (16), we obtain the auxiliary function $F(y, z)$:

$$(17) F(y, z) = 0.5 \left[k(y - a)^2 - c \cdot \cos(2\pi y) + k(z - a)^2 - c \cdot \cos(2\pi z) + 2b \right] + 0.5q(y - z)^2.$$

The motion to the minimum of the function $f(x)$ of two representative points with the initial values of the coordinates $y = 0$ and $z = 10$, belonging to the initial function (16), in accordance with the algorithm of the heavy ball method is shown in Fig. 4(b), of the gradient method - in Fig. 4(c).

To minimize the function (17) we'll apply the following methods: coordinate descent, gradient method with constant pitch and heavy ball method. Lines of the function level (17) with the motion path of representative points to its minimum, in accordance with the algorithms of the abovementioned methods (with $k = 0.2$, $a = 4$, $b = 3$, $c = 2$, and $q = 1$) are presented in Fig. 5-7.

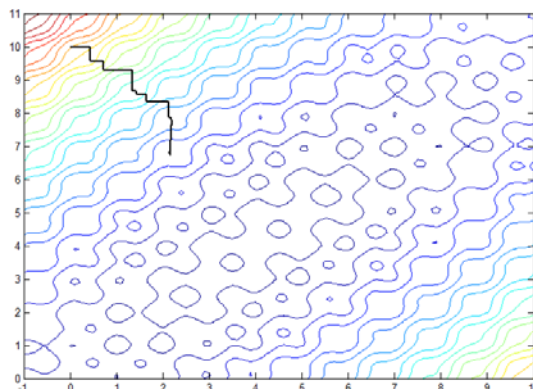


Fig. 5. Graphical illustration of the movement to a minimum by the coordinate descent method

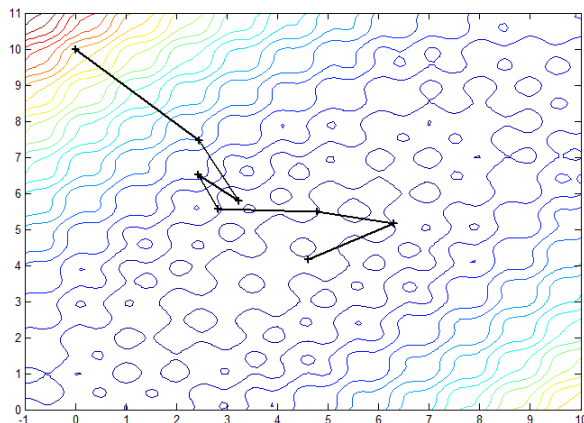


Fig. 6. Graphical illustration of the movement to a minimum by the gradient method with constant pitch

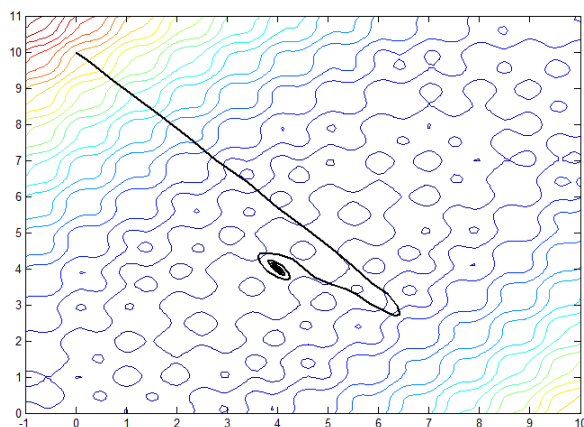


Fig. 7. Graphical illustration of the movement to a minimum by the heavy ball method

When the amplitude is increased in methods of coordinate descent and gradient descent with a constant pitch, the representative points end their motion in local extremums ($y = 6.8420$ and $z = 2.1491$ - coordinate descent method, $y = 4.1595$ and $z = 4.6124$ - gradient descent method with constant pitch). In the heavy ball method the process of motion of the representative points ends at the point of the global optimum $x^* = 4$. The calculated values were: $y = 4.0006$ and $z = 3.9973$, with a mass of heavy balls $m = 2.3$ and a damping factor $r = 2$.

4. Conclusion

The work of the algorithm of the modified heavy ball method, based on the principle of symmetry was investigated. The results of the research showed that for the test functions of Ackley, Griewank and Schwefel the seeking for a global extremum of a function using the usual heavy ball method does not give a positive result. However, the application of the concept of symmetry to the algorithm of the heavy ball method gave the desired result: the algorithms converge over time to the global minimum of multiextremal functions. When the amplitude of the oscillations of the multiextremal function (16) is increased, gradient methods of zero and first order are unsuitable for seeking for the global extremum of the function, since the representative points terminate at local minima. In addition, the considered algorithm of the heavy ball method with the application of the symmetry principle has good operability and high accuracy. Thus, the parallelization of the process of seeking for an extremum of a function based on the use of the concept of symmetry with regard to optimization problems will subsequently yield a number of positive results for estimating unknown parameters of objects in solving the problems of metrology of dynamic measurements and the synthesis of adaptive identification systems.

Bibliography

1. Стоян Б.Г. Решение некоторых многоэкстремальных задач методом сужающихся окрестностей / Б.Г. Стоян, В.З. Соколовский. – К.: Наук. думка, 1980. – 208 с.
2. Бахвалов Н.С. Численные методы (анализ, алгебра, обыкновенные дифференциальные уравнения) / Н.С. Бахвалов. – М.: Наука, 1973. – 632 с.
3. Васильев Ф.П. Численные методы решения экстремальных задач / Ф.П. Васильев. – М.: Наука, 1988. – 552 с.
4. Корсун В.И. Использование симметрии для распараллеливания процесса поиска экстремума целевой функции в задачах оптимального проектирования и адаптивной идентификации / В.И. Корсун // Математические модели и современные информационные технологии: сб. науч. тр. НАН Украины, Ин-т математики. – К.: 1998. – С.66-68.
5. Kharlamova Y.N. Study of the process of seeking global extremum of function by symmetric algorithms with parallel space / Y. N. Kharlamova, V.I. Korsun // Systems technologies — 2015. — № 5(100). — С. 151-161.
6. Korsun V. Paralleling of extremum seeking process in technical problems. / V. Korsun, Y. Harlamova // Science, Education and Culture in Eurasia and Africa: The 5th International Academic Congress (23-25 March 2015, Paris, France). – “Paris University Press”, 2015. – С. 112-116. – ISBN 978-2-547-75283-5.
7. Корсун В.И. Расширение возможностей методов установления при поиске глобального экстремума функции на основе концепции симметрии / В.И. Корсун, Ю.В. Жихарев, В.Л. Галюта // Матеріали міжнародної конференції «Математичні проблеми технічної механіки». – Д.: ДНВП «Системні технології», – 2005. – С.160.
8. Харламова Ю.Н. Оценка эффективности симметричного алгоритма метода тяжелого шарика при поиске глобальных экстремумов тестовых функций / Ю.Н. Харламова // Гірнича електромеханіка та автоматика – 2015. — №95 – С 31-35.

STABILITY ANALYSIS AND SIMULATIONS OF BIOREACTOR MODEL WITH DELAYED FEEDBACK

Assist. Prof., Ph.D. Borisov M.¹, Prof., Ph.D. Dimitrova N.¹, Prof., D.Sc. Krastanov M.^{1,2}
 Institute of Mathematics and Informatics, Bulgarian Academy of Sciences¹
 Faculty of Mathematics and Informatics, Sofia University, Bulgaria²

E-mail: milen_kb@math.bas.bg, nelid@math.bas.bg, krastanov@fmi.uni-sofia.bg

Abstract: We consider a well known mathematical model of continuous methane fermentation, consisting of two nonlinear ordinary differential equations and one algebraic equation for the gaseous output. The model involves one microbial population and one substrate. We propose an output feedback including a discrete delay and use it for asymptotic stabilization of the model. Feedback control of bioreactor models provides many advantages in operating a plant, mainly by increasing its efficiency. We also propose a numerical model-based extremum seeking algorithm for maximizing the biogas (methane) flow rate in real time. Numerical simulations using this algorithm are included. The simulations are implemented in the Python programming language which is recently recognized as a powerful modern general purpose object-oriented language.

Keywords: BIOREACTOR MODEL, DELAY FEEDBACK CONTROL, EXTREMUM SEEKING ALGORITHM

1. Introduction

We consider a well known mathematical model of the continuous methane fermentation, consisting of two nonlinear ordinary differential equations and one algebraic equation

$$\begin{aligned} \frac{ds}{dt} &= -k_1\mu(s)x + u(s_{in} - s) \\ \frac{dx}{dt} &= (\mu(s) - \alpha u)x \end{aligned} \quad (1)$$

with gaseous output

$$Q(s, x) = k_2 \mu(s)x, \quad (2)$$

where $x = x(t)$ and $s = s(t)$ are state variables, x is biomass concentration [g/dm³], s – substrate concentration [g/dm³], u – dilution rate [day⁻¹], s_{in} – influent substrate concentration [g/dm³], k_1 – yield coefficient [-], k_2 – coefficient [(dm³)²/g], Q – methane gas flow rate [dm³/day]. The parameter $\alpha \in (0, 1)$ represents the proportion of bacteria that are affected by the dilution; $\alpha = 0$ and $\alpha = 1$ correspond to an ideal fixed bed reactor and to an ideal continuous stirred tank reactor, respectively. The dilution rate u is considered as a control variable. The model function $\mu(s)$ represents the specific growth rate of the biomass.

Assumption A1. We assume that μ is defined for $s \in [0, +\infty)$, $\mu(0) = 0$ and $\mu(s) > 0$ whenever $s > 0$, $\mu(s)$ is continuously differentiable for all $s > 0$.

We propose here an output feedback including a discrete delay and use it for asymptotic stabilization of the dynamic model (1). Feedback control of bioreactor models provides many advantages in operating a plant and is used to increase its efficiency. On the other hand, there is always a time delay between input and output measurements in industrial and biological systems [4].

We make the following assumption.

Assumption A2. Assume that lower bounds s_{in}^- and k_2^- for the values of s_{in} and k_2 respectively, and an upper bound k_1^+ for the value of k_1 are known.

Denote for simplicity

$$\beta^- = \frac{k_1^+}{k_2^- s_{in}^-}.$$

Define the following feedback control law:

$$k(s, x) = \beta k_2 \mu(s)x \text{ with } \beta \in (\beta^-, +\infty).$$

Replacing in the model (1)–(2) u by the feedback

$$k(s(t - \tau), x(t - \tau)),$$

where $\tau > 0$ is a discrete delay, we obtain the following control system:

$$\frac{ds}{dt} = -k_1\mu(s(t))x(t) + \beta k_2\mu(s(t - \tau))x(t - \tau)(s_{in} - s(t)) \quad (3)$$

$$\frac{dx}{dt} = \mu(s(t))x(t) - \alpha\beta k_2\mu(s(t - \tau))x(t - \tau) \quad (4)$$

Choose some $\beta \in (\beta^-, +\infty)$ and let

$$\bar{s} := s_{in} - \frac{k_1}{k_2\beta} \quad (5)$$

Obviously, $\bar{s}$ belongs to the interval $(0, s_{in})$. Define

$$\bar{x} := \frac{1}{\alpha\beta k_2} \quad (6)$$

It is straightforward to see that the point

$$\bar{p}_\beta := (\bar{s}, \bar{x})$$

is an equilibrium point for (3)–(4).

2. Stability analysis of the model

Assumption A3. We assume that the following inequalities hold true

$$\mu(s^-) < \mu(\bar{s}) < \mu(s^+)$$

for each $s^- \in (0, \bar{s})$ and $s^+ \in (\bar{s}, s_{in})$.

Assumption A3 is technical. It is always fulfilled when the function $\mu(s)$ is monotone increasing (like the Monod specific growth rate, see Section 4). If the function $\mu(s)$ is not monotone increasing (like e. g. the Haldane law) then the point $\bar{s}$ (i.e. β) has to be chosen in a proper way in order to satisfy Assumption A3.

Below we present a result about the local asymptotic stability of the equilibrium point $\bar{p}_\beta$ with respect to the parameters of the closed-loop system (3)–(4). Denote for simplicity:

$$\begin{aligned} b &= k_1 \bar{x} \mu(\bar{s}) \mu'(\bar{s}) \\ d &= \mu(\bar{s}) \left(\frac{1}{\alpha} \mu(\bar{s}) - k_1 \bar{x} \mu(\bar{s}) \right) \end{aligned}$$

where the coefficients b and d depend on the parameter β , since $\bar{s}$ and $\bar{x}$ are functions of β , see (5) and (6).

Theorem 1.

(i) If $b \geq d$ then the equilibrium point $\bar{p}_\beta$ is locally asymptotically stable for any value of the delay $\tau > 0$.

(ii) If $b < d$ then there exists a delay $\tau_0 > 0$ such that the equilibrium point $\bar{p}_\beta$ is locally asymptotically stable for all values τ of the delay such that $\tau < \tau_0$; the equilibrium is locally unstable if $\tau \geq \tau_0$, and a Hopf bifurcation occurs at $\tau = \tau_0$.

The proof of the theorem is rather long and will not be presented here due to the restricted paper length. The proof is based on some ideas from [3], [5] and [6].

We suppose that in the cases when the equilibrium point $\bar{p}_\beta$ is locally asymptotically stable then it is also globally asymptotically stable. The computer simulations confirm that assumption (see Section 4). Proving global stability of $\bar{p}_\beta$ will be a subject of further studies.

3. Maximizing the biogas production via extremum seeking

Consider the equation (2) describing the process output, i.e. the methane (biogas) production. In this section we shall shortly present a numerical extremum seeking algorithm (ESA), cf. [1]–[2], to steer and stabilize the dynamics (3)–(4) towards a steady state, where maximum methane flow rate Q_{max} is achieved. For that purpose we compute Q on the set of all equilibrium points, parameterized with respect to β . Denote the so obtained function by $Q(\beta)$, where $\beta \in (\beta^-, +\infty)$. The function $Q(\beta)$ is called input-output static characteristic of the model. Assume that the function $\beta \rightarrow Q(\beta)$, $\beta \in (\beta^-, +\infty)$, is strongly unimodal, i.e. there exists a unique point $\beta_{max} \in (\beta^-, +\infty)$ where $Q(\beta)$ takes a maximum, $Q_{max} = Q(\beta_{max})$, the function strongly increases in the interval (β^-, β_{max}) and strongly decreases in $(\beta_{max}, +\infty)$.

Let

$$p_{\beta_{max}} = (\bar{s}_{max}, \bar{x}_{max})$$

be the steady state where Q_{max} is achieved. Our goal is to stabilize in real time the system (3)–(4) towards this (unknown) equilibrium point $p_{\beta_{max}}$ and therefore to the maximum methane flow rate Q_{max} .

The main idea of ESA is the following: we construct a sequence of points $\beta^1, \beta^2, \dots, \beta^n, \dots$ from the interval $(\beta^-, +\infty)$, each β^j being in the form $\beta^j = \beta^{j-1} \pm h$, $h > 0$, and such that the sequence $\{\beta^j\}$ tends to β_{max} . Then by computing and comparing the values $Q(\beta^1), Q(\beta^1), \dots, Q(\beta^n), \dots$, we achieve the desired equilibrium point $p_{\beta_{max}}$ and thus Q_{max} .

In the computer implementation ESA is carried out in two stages. In the first stage, “rough” intervals $[\beta]$ and $[Q]$ are found which enclose β_{max} and Q_{max} respectively; in the second stage, the interval $[\beta]$ is refined using an elimination procedure based on the golden mean value (or Fibonacci search) strategy. The second stage produces the final intervals $[\beta_{max}] = [\beta_{max}^-, \beta_{max}^+]$ and $[Q_{max}]$ such that $\beta_{max} \in [\beta_{max}]$, $Q_{max} \in [Q_{max}]$ and $\beta_{max}^+ - \beta_{max}^- \leq \varepsilon$, where the tolerance $\varepsilon > 0$ is specified by the user.

The ESA was firstly developed for the model (3)–(4) with $\tau = 0$, cf. [1], [2]. Now the algorithm is modified for the delayed model and is implemented in the object-oriented language *Python*. Nowadays, this programming language has become an integral part of scientific and engineering computing due to the vast abundance of open source libraries and interfaces to major software tools.

4. Numerical Simulation

In the simulation process we consider the Monod specific growth rate

$$\mu(s) = \frac{m_1 s}{k_s + s},$$

where m_1 is the maximum specific growth rate of the microorganisms [1/day] and k_s is the saturation constant [g/dm³].

We use the following numerical values for the model parameters (cf. [1] and the references therein):

$$k_1 = 27.4, s_{in} = 3, m_1 = 0.4, k_s = 0.4, \alpha = 0.5, k_2 = 75.$$

With $k_1^+ = 27.6$, $s_{in}^- = 2.8$ and $k_2^- = 74.8$ we obtain that $\beta^- = \frac{k_1^+}{s_{in}^- k_2^-} \approx 0.1318$. Therefore the parameter β varies in the interval $(0.1318, +\infty)$.

For the above parameter values, the input-output static characteristic $Q(\beta)$ is strongly unimodal and takes its maximum for $\beta = \beta_{max} = 0.16355$ (see Figure 1), thus $Q_{max} = 3.21376$, $\bar{s}_{max} = 0.76619$ and $\bar{x}_{max} = 0.16305$.

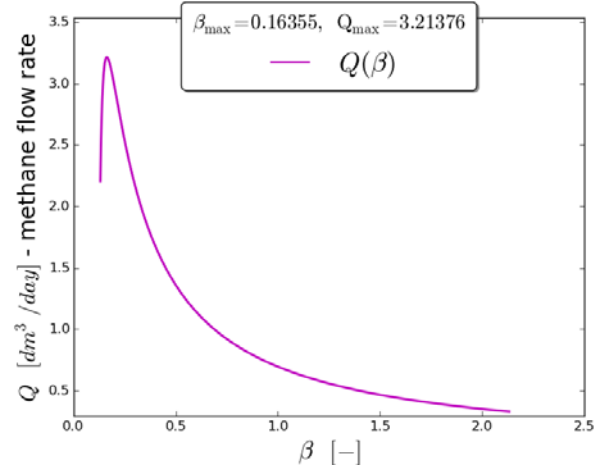


Fig. 1. The input-output static characteristic $Q(\beta)$

4.1. Simulation of the global dynamics behavior

First we shall demonstrate numerically the stability of the system (3)–(4) towards the equilibrium point $\bar{p}_\beta$ for different values of the delay τ and the parameter β .

(i) $\beta = \beta_{max} = 0.16355$

For this value of β , the inequality $b > d$ is fulfilled. According to Theorem 1, the equilibrium point $(\bar{s}_{max}, \bar{x}_{max}) = (0.76619, 0.16305)$ is stable for any $\tau \geq 0$ as it can be seen in the Figures 2 to 4 for the following values of the delay: $\tau = 1$, $\tau = 5$ and $\tau = 15$.

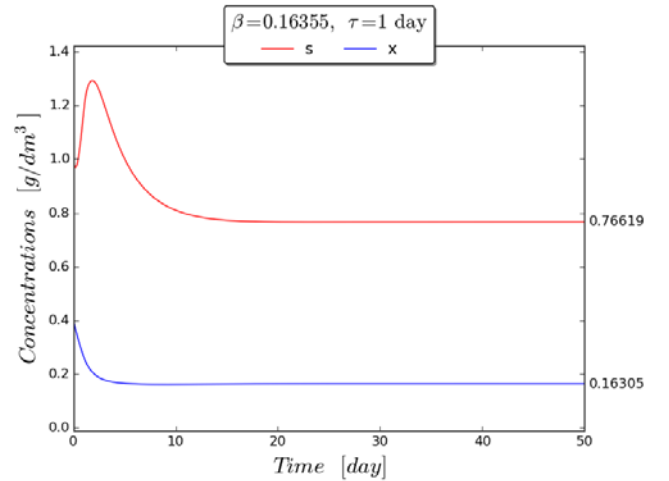


Fig. 2. $\beta = \beta_{max} = 0.16355$, $\tau = 1$: Time evolution of s and x towards $\bar{s}_{max}$ and $\bar{x}_{max}$ respectively

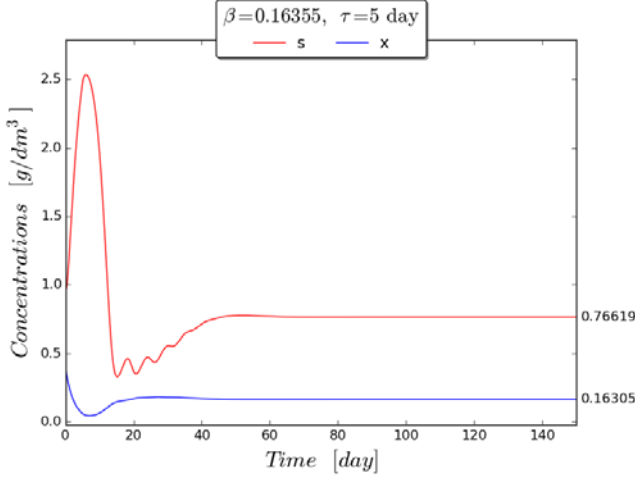


Fig. 3. $\beta = \beta_{\max} = 0.16355$, $\tau = 5$:
Time evolution of s and x towards $\bar{s}_{\max}$ and $\bar{x}_{\max}$ respectively

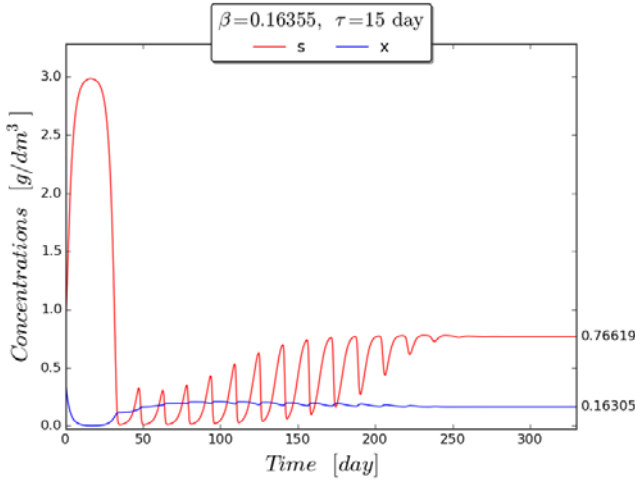


Fig. 4. $\beta = \beta_{\max} = 0.16355$, $\tau = 15$:
Time evolution of s and x towards $\bar{s}_{\max}$ and $\bar{x}_{\max}$ respectively

(ii) $\beta = 1.0$

Here $b < d$ is valid. In this case $\tau_0 = 4.70326$, $\bar{s} = 2.63467$ and $\bar{x} = 0.02667$. According to Theorem 1, the equilibrium point $(\bar{s}, \bar{x})$ is stable for any $\tau < \tau_0$ and unstable for any $\tau \geq \tau_0$; this is demonstrated in Figures 5 to 8 when the delay takes the values $\tau = 1$, $\tau = 4.5$, $\tau = 5$ respectively.

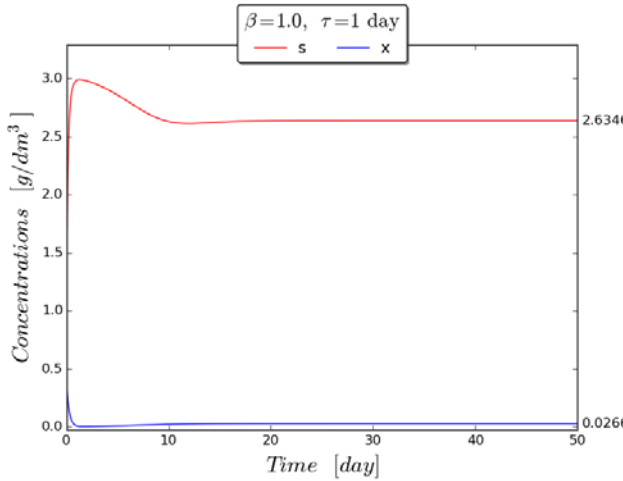


Fig. 5. $\beta = 1$, $\tau = 1$: Time evolution of s and x towards $\bar{s}$ and $\bar{x}$

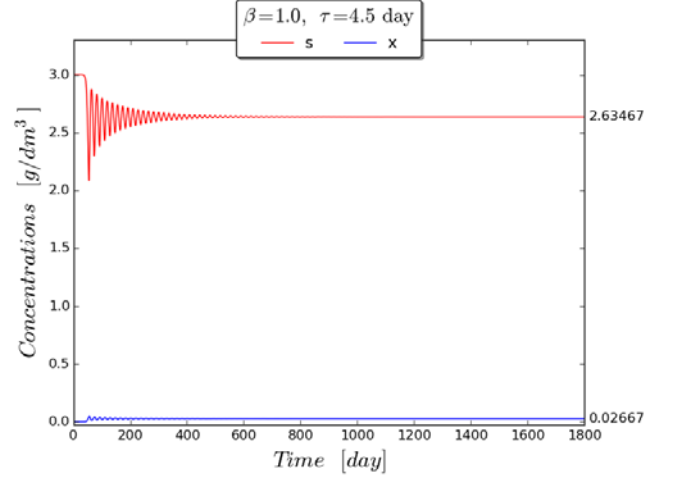


Fig. 6. $\beta = 1$, $\tau = 4.5$: Time evolution of s and x towards $\bar{s}$ and $\bar{x}$

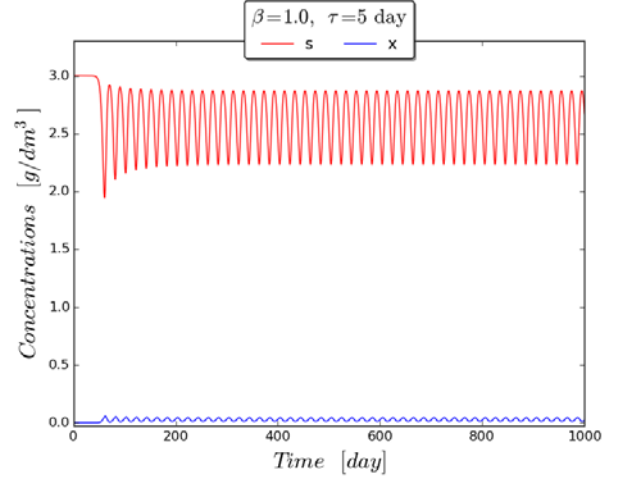


Fig. 7. $\beta = 1$, $\tau = 5$: Time evolution of s and x towards $\bar{s}$ and $\bar{x}$

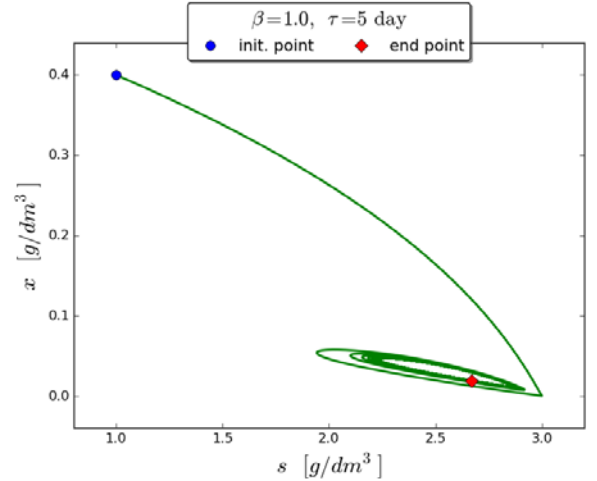


Fig. 8. $\beta = 1$, $\tau = 5$: A trajectory in the phase plane (s, x)
Existence of a periodic solution as a result of Hopf bifurcation

The graphic visualizations (see Figures 2 and 5), as well as other simulations, that are not presented in the paper, show that for a delay $\tau = 1$ [day] the dynamics is stabilized approximately within 10 days, which is practically reasonable for the modeled process. Increasing the delay leads to the appearance of damped oscillations and the time for the solution stabilization increases (see Figures 3 and 6 for $\tau = 5$ and $\tau = 4.5$ respectively). For extremely large (and practically unusual) value of the delay ($\tau = 15$ [days] in Figure 4), as well as for $\tau \geq \tau_0$ (e.g. $\tau = 5$ [days] in Figures 7 and 8) sustainable oscillations do occur.

4.2. Simulation results from the extremum seeking algorithm

The numerical results from the extremum seeking algorithm (ESA) are visualized in Figures 9 to 12 for small values of the delay $\tau = 1$ and $\tau = 3$.

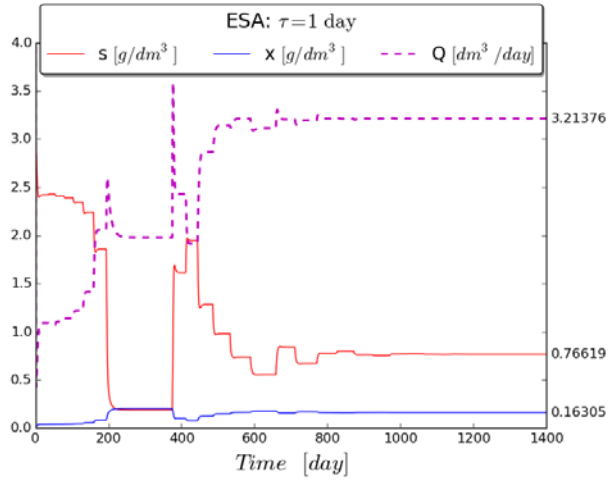


Fig. 9. $\tau = 1$. Visualization of the numerical results from the ESA. Time evolution of s, x and Q towards $\bar{s}_{max}$, $\bar{x}_{max}$ and Q_{max}

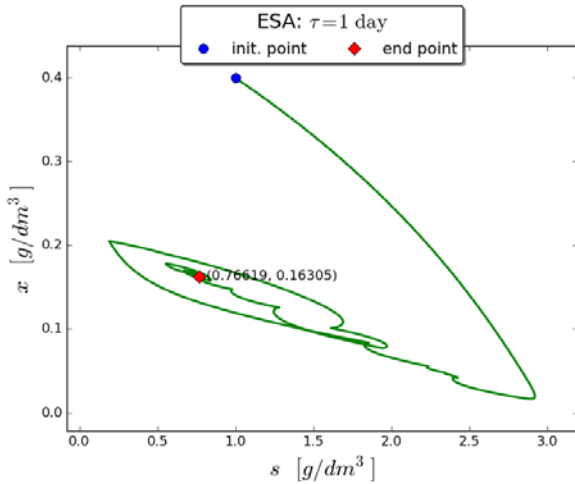


Fig. 10. $\tau = 1$. Visualization of the numerical results from the ESA. A trajectory in the phase plane (s, x) .

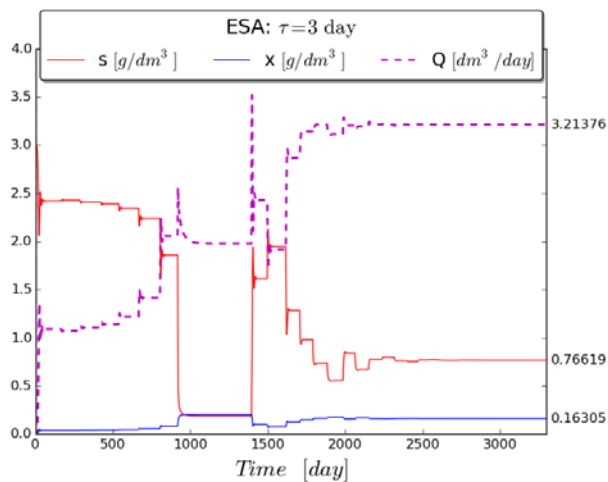


Fig. 11. $\tau = 3$. Visualization of the numerical results from the ESA. Time evolution of s, x and Q towards $\bar{s}_{max}$, $\bar{x}_{max}$ and Q_{max}

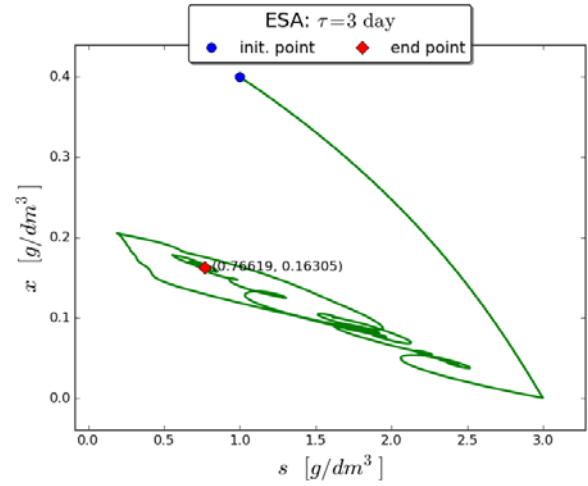


Fig. 12. $\tau = 3$. Visualization of the numerical results from the ESA. A trajectory in the phase plane (s, x) .

5. Conclusion

In this paper we investigate a nonlinear functional-differential model of an anaerobic bioreactor with methane (biogas) production, involving one microbial population and one substrate. The stabilization of the model solutions is carried out by a feedback control law involving one discrete time delay. We have established local asymptotic stability of the system dynamics towards a previously chosen equilibrium point as well as bifurcations of this equilibrium with respect to the time delay. The numerical simulations suggest that in the cases when the equilibrium point is locally asymptotically stable it is also globally stable. This allows us to apply a numerical model-based extremum seeking algorithm for stabilizing the dynamics towards the equilibrium point where maximum production of methane is achieved. The facilities of the algorithm are illustrated numerically as well.

Acknowledgements

The research of the first and the second author has been supported by the Bulgarian Academy of Sciences, Program for Support of Young Scientists and Scholars, grant № DFNP-17-25/25.07.2017. The work of the second and the third author has been partially supported by the Sofia University "St. K. Ohridski" under grant № 80-10-220/22.04.2017.

References

- [1] N. Dimitrova, M. Krastanov: Nonlinear Adaptive Control of a Model of an Uncertain Fermentation Process. *Int. Journ. Robust Nonlinear Control*, 20, 1001–1009, 2010.
- [2] N. S. Dimitrova, M. I. Krastanov: Adaptive Asymptotic Stabilization of a Bioprocess Model with Unknown Kinetics. *Int. J. Numerical Analysis and Modeling, Series B, Computing and Information*, vol. 2, No. 2–3, 200–214, 2011.
- [3] Y. Kuang: *Delay Differential Equations with Applications in Population Dynamics*. Academic press, 1993.
- [4] G. Robledo: Feedback Stabilization for a Chemostat with Delayed Output. Preprint INRIA Sophia Antipolis RR No 5844, 2004.
- [5] S. Ruan: On Nonlinear Dynamics of Predator-Prey Models with Discrete Delay. *Math. Model. Nat. Phenom.* 4 (2), 140–188, 2009.
- [6] H. Smith: *An Introduction to Delay Differential Equations with Applications to the Life Sciences*. Springer, 2011.

INVESTIGATION OF SAMPLES ACCURACY TO MODEL THE PROCESSES IN 3D PRINTING

Assoc. Prof. MEng. Minev R. PhD., Assoc. Prof. MEng. Rusev R. PhD., MEng. Antonov S. PhD., MEng. Minev E. PhD.
"Angel Kanchev" University of Ruse, Bulgaria

eminev@uni-ruse.bg

Abstract: 3D printing also called Layer based technology, Freeform fabrication, Additive manufacturing or Rapid Prototyping technologies has undergone significant development over the last decades. The growth is related to the expansion of the range of materials used, application areas, and range of possible sizes from nanometer to tens of meters as well as increasing machine accessibility. There is a growing consensus that 3D printing technologies will be at the heart of the next major technological revolutions. At present there are some technological specifics and associated difficulties in 3D printing one of which is the accuracy of the manufactured product. Research in this area would allow modelling of 3D printing processes.

The article describes the possible types and sources of inaccuracies in 3D printing processes. The various types of test pieces used in practice are examined to quantify the errors in shape and sizes after building. Test pieces with predefined discrete points and methodology are provided to calculate inaccuracies. The results are presented in the terminology of "linear" and "shear" deformations. This gives opportunity to determine the variations in the shape and dimensions of the parts built by 3D printing. On the basis of the discrete results obtained, the possibility of 3D printing process modelling is discussed and presented.

Keywords: 3D PRINTING, ACCURACY, MODELLING, TEST PART, GRID METHOD

1. Introduction

Additive Manufacturing (AM or commonly known as 3D printing and before that rapid prototyping - RP) undergone significant development during the past decades in terms of production volume and technological achievements. However the AM industry only began to grow substantially after 2009 probably because the last major AM patent for Fused Deposition Modeling (FDM) expired in 2009. This way 3D printers could be produced without infringing on intellectual property, creating a newfound interest and investment in 3D printing [1]. This is particularly valid for the introduction of affordable consumer 3D printers into the general market on the basis of so-called RepRap (affordable open source replicating rapid prototyper). Hence the main drivers for the rapid growth are the reduction in cost to access the technology, an increase in applications [2] as well as expanding of the range of materials used and printed dimensions. Additive manufacturing has been called a disruptive technology [3] that will fundamentally influence many processes in production. Predicting of the future of AM on economic and social implications is constantly on the focus of the researchers [4, 5] and companies [6]. There is a growing consensus that 3D printing technologies will be one of the next major technological revolutions [7].

Although AM is a breakout technology, the implementation of it is still in infancy. There are numerous challenges in applying AM. One major obstacle is lower accuracy relative to other technologies [2]. The errors in sizes and shapes of produced component reflect various reasons during the build up stage. A possible general classification of error sources common for most popular AM processes comprises the following [8]: errors caused by laser scanning system; errors caused by material shrinkage; errors caused by spot size and heat effected zone; errors caused by Computer Aided Design (CAD), tessellation and slicing; random errors. The thermal nature of most of the process leads to shrinkage, distortion and warping of the built part. All of these factor can contribute to significant errors in the final component. Therefore it is especially important to perform an accuracy analysis that systematically reveals the type of errors, their sources and magnitudes, so that improvements in the production practice can be implemented. If enough data about accuracy of a given process is gathered, the process can be modeled in terms of its accuracy performance.

2. Prerequisites and means for solving the problem

The manufacturing parameters in AM have great significance on the part integrity, strength, density, surface quality and shrinkage for different processes and materials. The analysis of process parameters is therefore one of the main streams of RP research.

Once an optimum set of parameters are established they are kept as a material's "profile". In particular cases of unexpected changes to part quality, adjustments to the parameters can be made according to the experience of the machine operator or platform manufacturer recommendations. In most cases of AM it is practical to set the build parameters for optimum part strength, surface quality and build time. On this basis the accuracy in size and shape of the part can be targeted by applying scaling factors, beam offset compensation, part orientation and arrangement in the building chamber. As the manufacturing conditions at different areas of the build chamber vary, the overall accuracy of the process or platform is not uniform. The research in [9, 10] (Fig. 1) shows that the temperature variations of a SLS machine are considerable. It can be expected that the differences in shrinkage to room temperature and the ultimate accuracy of the build part will reflect these variations.

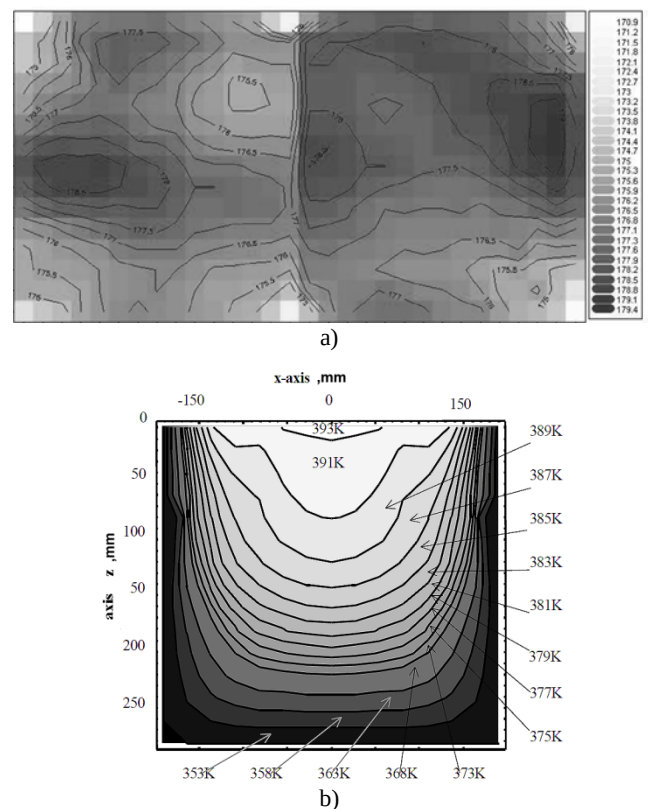


Fig. 1. Temperature distribution in the part bed - a) reported by [9] and b) reported by [10].

Essentially the practice of accuracy research in AM requires the building of various test parts or series of parts and evaluating the differences between their nominal and actual dimensions and shapes. Linear and angular dimensions, point's coordinates and surface roughness are the basic entities that are used to assess part geometry.

The elements that distinguish between different methodologies for accuracy studies of RP processes are test parts and the related measured geometrical entity. The most common types of test pieces can be classified as: pyramids (staircase); specifically designed parts; real parts. Typical examples of these are shown in fig. 2.

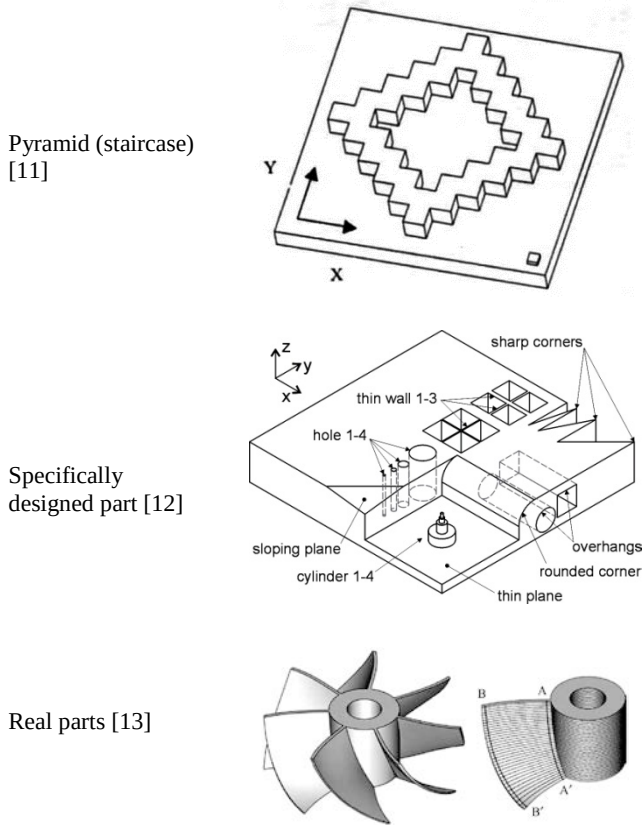


Fig. 2. Typical examples of test parts.

One of the drawback of all test pieces is that they don't cover entire surface of the part bed. Additionally they usually cross areas with different temperatures or with other manufacturing variations. As a result a continuous distribution of accuracies cannot be achieved. In case of the most popular type of test part - pyramid, the methodologies for accuracy investigation are based on measurements of the staircase dimensions and calculation of the material shrinkage in x, y or z direction. The measurements m_i are shown on fig. 3.

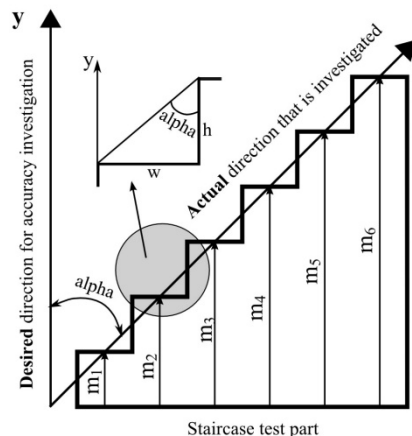


Fig. 3. Lengths and directions for measurements of pyramid shape test part.

The idea of such measurements is usually to determine the difference between the nominal dimension l_n and the final dimension l_f (produced by the machine) usually called the error (E):

$$E = L_f - L_n$$

The distribution of the errors E varies over the part bed defined as a plane (x, y). Geometrically the error is a function of two variables x and y :

$$E = f(x, y)$$

As illustrated in fig. 3, the direction in which the pyramid stairs advance is the "actual direction" defined by the angle α :

$$\alpha = \tan^{-1} \left(\frac{w}{h} \right)$$

This may not necessarily be the "desired direction" for investigation. Failure to observe this correctly can result in misleading directional results, particularly if z direction is investigated by vertical pyramid - fig. 4.

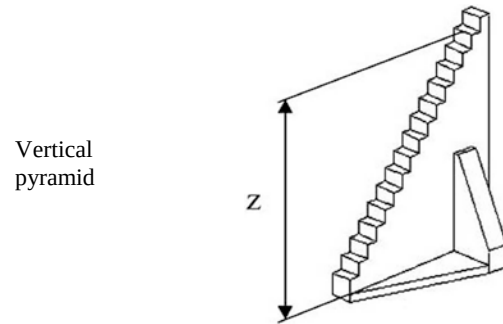


Fig. 4. Vertical pyramid for z accuracy investigation.

The most common approach of using the pyramid type of test piece is to compare the nominal (as in CAD model) and actual size of the steps as shown in fig. 5 [14]. The comparison of the results in coordinates "nominal dimensions - actual dimensions" is represented by an interpolation graph which slope is interpreted as the scaling factor. It has to be applied to the CAD model in order to achieve closer real part dimensions to the nominal. The intercept that the interpolation line cuts from the vertical coordinate axis of the graph gives the size of the systematic error due to the size of the extruded plastic jet or laser beam spot.

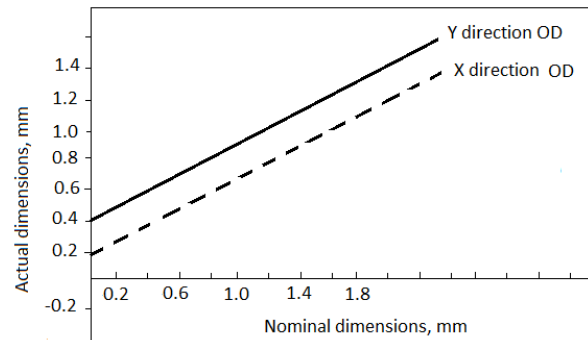


Fig. 5. Linear interpolation "nominal size - actual size" of the outside (OD) in X and Y direction of the pyramid.

In general practice it is important to know the length changes either in any directions or in some particular directions. In order to model the total accuracy of the AM process or specific platform or material behaviour in terms of shrinkage, constructing a map of entire field of distortions is essential. It is not achievable by utilising the test parts and measurement approach described above.

3. Solution of the examined problem

Regardless of the cause, it can be assumed that the change of dimensions or shape of a body manifests itself in the same geometrical appearance as strain. Strain is defined as being linear (ϵ) or angular (γ). The angular change in a right angle, known as

shear strain, is defined as the change in angle between two line segments which were previously mutually perpendicular. An advantage of describing the inaccuracy of parts manufactured by AM processes in terms of strains, is the possibility it allows to combine analysis of dimensional and shape deviation from nominal.

The analysis methodology that is proposed in this study for accuracy modeling of AM processes is based on measurement of coordinates x , y or z at many points throughout a test piece in the form of a flat plate. To expose the strains, a reference grid in some form is applied to the CAD model of the test piece beforehand. After the plate is manufactured the actual coordinates of grid points is measured and compared with the CAD model. As the produced grid differs from the nominal CAD grid it can be considered as deformed and therefore the strains calculated. Several ways to estimate the strains of a deformed object are known however the Coefficient or Square Grid Method is utilised here. This method was introduced by Bredendick in [15, 16].

The advantage of such a methodology is the simple geometry of the test part - a plate with reference points in form of hole, cross or other spot mark. The plate can be arbitrary in size, location and orientation within the build chamber (fig. 6). It is also suitable for handling and automatic measuring as well as being representative of various engineering parts.

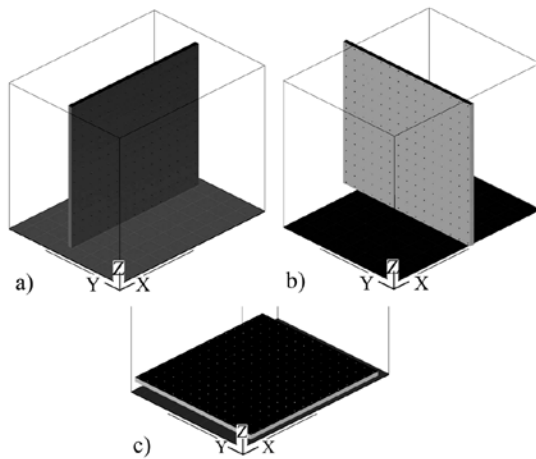


Fig. 6. Examples of test plate orientation.

If the plate is built horizontally the deviations ϵ_x and ϵ_y (fig. 6c) can be determined, if positioned vertically then either ϵ_z and ϵ_x (fig. 6a) or ϵ_z and ϵ_y (fig. 6b) can be calculated together with associated angular strains - γ_{xy} , γ_{zx} , γ_{zy} . By building a set of plates with a given orientation and in different positions in the build chamber, a three dimensional concept and model of the distribution of dimensional deviations over the entire build envelope can be created - fig. 7.

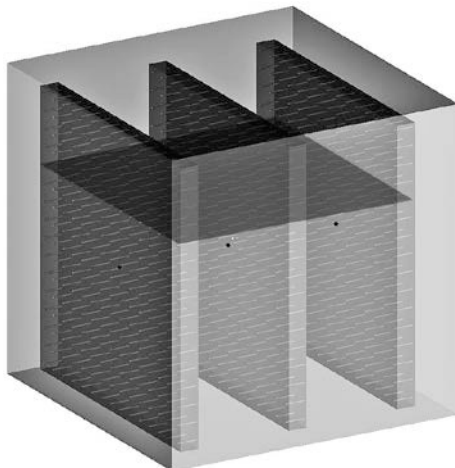


Fig. 7. Set of test parts for 3D concept and model of the accuracy distribution.

Accumulating a data from experimental set up similar to that shown on fig. 7 will allow interpolations of deformations from plates oriented in ($z - y$) to other directions by combining the points from different plates and forming virtual plates in perpendicular direction - the transverse surface on fig. 7.

4. Results and discussion

The experimental test plate was built by Selective Laser Sintering (SLS) process on DTM 2500 *Plus* machine according the settings on fig. 6a. The material used was polystyrene Castform. The hole centres was measured routinely by coordinate measuring machine (CMM) Mitutoyo QuickVision *Pro*. For that purpose a specialised software was developed that allows, together with Mitutoyo software, the total measurement to be done within minutes after the initial datum point and axis are set. The setting and the screenshot of the measuring software action are shown in fig. 8.

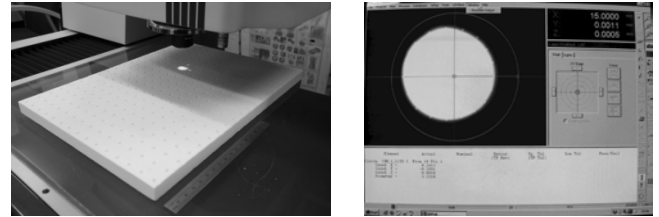


Fig. 8. Plate measuring process and screen shot of software window.

The accumulated data of x and y coordinates of grid points as holes is used as input data for linear and angular deviations from nominal calculations. For this purpose a VBA program for MS Excel spreadsheet was developed. The next step in data processing includes a MatLab program that was developed to analyse the results and to generate a 3D visualisation of the distributions of linear and shear deformations over the test part surface. The results are shown on fig. 9 and fig. 10.

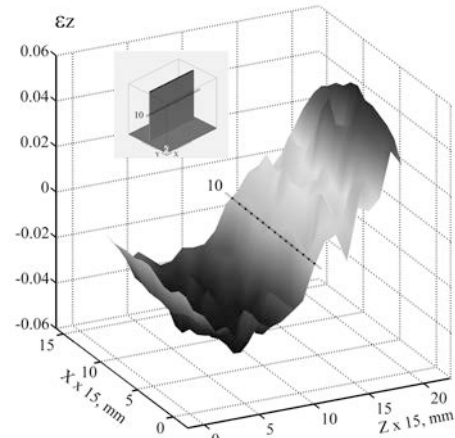


Fig. 9. 3D visualisation of ϵ_z (vertical size deviations from nominal) distribution in the (x , z) plane.

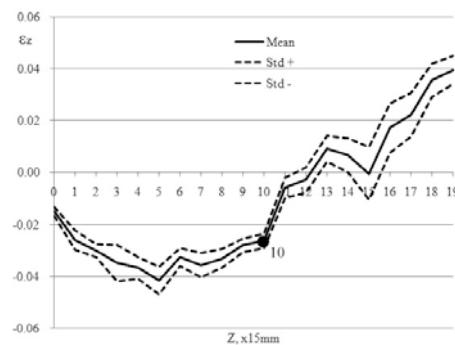


Fig. 10. Distribution of ϵ_z -vertical deviation of the sizes from nominal.

The mean value of all reference points along each row of the plate gives a point of the line shown on fig. 10. As an example the highlighted row "10" from fig. 9 gives the position of the point "10" on the fig. 10.

The results show that a single test piece and routine measurement procedure can be utilised to estimate the distribution of linear and angular deviations from the nominal sizes of AM parts. The geometry of the utilised test piece has advantages over the stair case (pyramid) type test pieces since it gives correct data about inaccuracy distribution along a particular direction or particular axes. The routine automatic measurements and data processing are possible due to the simple geometry of the samples and feasible software development.

5. Conclusion

Some estimates about accuracy of a process or platform can be done even with a single test piece. As it can be seen from fig. 9 and fig. 10 the described methodology can present the continuous distribution of distortions described in terms of linear and angular strains which can be interpreted as deviations from nominal in size and shape.

The data connection from several plates by interpolations is a step forward that can allow modelling of the entire build envelope, process or material accuracy. For that purpose a sufficient number of test plates over the entire build volume has to be produced and analysed.

The modelling of distribution of deviations from nominal, creates a possibility to reduce these deviations. One approach is a pre-deformation of the part data contrary to the expected defect. This can be implemented by using a free-form deformation (FFD) approach [17]. The FFD deforms the surrounding cuboid of an object in order to adapt the embedded object. Thus, an increased size and shape accuracy can be achieved by choosing suitable parameters for the FFD.

References

1. Van Lancker, P., 3D Printing: The Influence of Intellectual Property. CREAX, 12 August 2015. <https://www.creax.com/en/our-work/the-3d-printing-evolution-insights-on-the-influence-of-ip-on-technology-dev> (accessed 29/11/2017).
2. Attaran, M., Additive Manufacturing: The Most Promising Technology to Alter the Supply Chain and Logistics. *Journal of Service Science and Management*, 10, 2017, 189-205.
3. Petrick, I. J., T. W. Simpson, 3D printing disrupts manufacturing: how economies of one create new roles of competition. *Res. Technol. Manag.*, 56 (6), 2013, 12-16.
4. Ford, S., M. Despeisse, Additive manufacturing and sustainability: an exploratory study of the advantages and challenges. *Journal of Cleaner Production*, 137, 2016, 1573-1587.
5. Jiang, R., R. Kleer, F. T. Piller, Predicting the future of additive manufacturing: A Delphi study on economic and societal implications of 3D printing for 2030. *Technological Forecasting & Social Change* 117, 2017, 84-97.
6. Wohlers Report, 3D Printing and Additive Manufacturing State of the Industry Annual Worldwide Progress Report, <https:// Wohlersassociates.com/2013contents.htm> (accessed 26/11/2017).
7. Thierry, R., L. Striukova, From rapid prototyping to home fabrication: How 3D printing is changing business model innovation. *Technological Forecasting & Social Change*, 102, 2016, 214-224.
8. Tang, Y., H. T. Loh, J. Y. H. Fuh, Y. S. Wong, L. Lu, Y. Ning, X. Wang, 2004. Accuracy analysis and improvement for direct laser sintering. *Innovation in Manufacturing Systems and Technology (IMST) 01*, <http://hdl.handle.net/1721.1/3898> (accessed 26/11/2017).
9. Shwe, P., S., Quantitative analysis on SLS part curling using EOS P700 machine. *Journal of Materials Processing Technology*, Volume 212, Issue 11, November 2012, Pages 2433-2442.

10. Shen, J., J. Steinberger, J. Göpfert, R. Gerner, F. Daiber, K. Manetsberger, S. Ferstl, Inhomogeneous shrinkage of polymer materials in selective laser sintering. *Proceedings of Solid Freeform Fabrication Symposium*, 2000, Austin, Texas, pp. 298-305.
11. DTM Corporation, 1999. The Sinterstation System, Guide to Materials: CastForm PS. DCN: 8002-10006.
12. Kruth, J. P., B. Vandenbroucke, J. Van Vaerenbergh, P. Mercelis, Benchmarking of different SLS/SLM processes as rapid manufacturing techniques. *International Conference of Polymers & Moulds Innovations*, April 20-23, 2005, Gent, Belgium, pp.1-7.
13. Jiang Cho-Pei, Development of a novel two-laser beam stereolithography system. *Rapid Prototyping Journal*, 2011, 17 (2), pp. 148-155.
14. Minev E., E. Yankov, R. Minev, The RepRap Printer for Metal Casting Patternmaking - Capabilities and Application. *Труды VIII Международной научно-практической конференции „Прогрессивные литейные технологии“*, НИТУ МИСиС, 16-20.11.2015, Москва, стр.300-303, ISBN 978-5-9903239-3-3.
15. Bredendick, F., Zur ermittlung von deformationen an verzerrten gittern. *Wiss. Technical University Dresden*, 1967, v. 16, pp. 1473-1481.
16. Bredendick, F., Zur ermittlung von deformationen an verzerrten gittern. *Wiss. Technical University Dresden*, 1969, v. 16, pp. 1473-1481.
17. Schmutzlera, C., A. Zimmermannb, M. F. Zaeha, Compensating warpage of 3D printed parts using free-form deformation. *48th CIRP Conference on Manufacturing Systems - CIRP CMS 2015. Procedia CIRP* 41, 2016, 1017 – 1022.

ELECTRIC POWER SYSTEMS MODELING AND EDUCATION: THE CONTROLLABLE LOADS IN A SHORT TERM SYSTEM BALANCE

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

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

Abstract: In this paper we try to build a framework in active power optimization model building when controllable loads are available for balancing purposes. A certain classification of non-fixed loads is given as well as the respective variables and constraints that have to be introduced in the mixed-integer linear programming model. A numerical example is also given illustrating the modeling approach. Some analysis on the presented numerical data is done in order to show sensitivity to certain environmental issues.

Keywords: OPTIMIZATION MODELING, ELECTRIC POWER SYSTEMS OPTIMIZATION, CONTROLLABLE LOADS

1. Introduction

When a load can be switched on or off when needed for system balance purposes, it is considered as a controllable load. An example of a controllable load in an EPS from the System's Operator point of view is the pumping capacities of an PHPS or a group of consumers whose power supply can be interrupted (and / or restricted) during peak load periods. For a micro-grid, a controllable load can be any consumer whose power can be managed and / or limited or its performance may be postponed (dispatched) over time. There are many loads whose operation extends over several time intervals. In this case for those loads is said that they have a working cycle. Since there are many possibilities in the handling of the controllable loads with a work cycle, it is necessary to introduce a certain classification for modeling purposes of such loads.

2. Loads classification and modeling framework

Type I. Controllable loads over time with an interruptible work cycle: These loads are assumed to have a fixed work cycle duration d_{l1*} and a fixed power level P_{l1*} in a single interval. The operation modeling of these loads requires the introduction of binary variables $v_{l1,j}$ having *true* value ($v_{l1,j} = 1$) when the load is switched to power level P_{l1*} in the interval j . Additions of the form $v_{l1,j}P_{l1*}$ must be introduced in the balance constraints. A constraint (1) handles the duration of the work cycle:

$$\sum_j v_{l1,j} = d_{l1*} \quad (1)$$

Type II. Controllable loads over time and consumption with an interruptible work cycle: The power consumed by this load $P_{l2,j}$ in the single interval j depends on the duration of the operating cycle $d_{l2}^{\min} \leq d_{l2} \leq d_{l2}^{\max}$. The total load consumption P_{l2}^{Σ} is known for a full work cycle. So the hour consumption $P_{l2,j}$ and the duration of the duty cycle d_{l2} are optimized introducing binary variables $v_{l2,j} = 1$ when the load is switched to power $P_{l2}^{\min} \leq P_{l2,j} \leq P_{l2}^{\max}$. In the latter the interval's limits are derived via: $P_{l2}^{\min} = P_{l2}^{\Sigma} : d_{l2}^{\max}$ and $P_{l2}^{\max} = P_{l2}^{\Sigma} : d_{l2}^{\min}$. Only the load consumption $P_{l2,j}$ is included in the balance constraint. For modeling the rest of the requirements, including the dependence between the cycle duration and the power level in the unit interval the following constraints are added:

$$P_{l2,j} - v_{l2,j} P_{l2}^{\max} \leq 0 \text{ and } P_{l2,j} - v_{l2,j} P_{l2}^{\min} \geq 0 \quad (2)$$

$$\sum_j v_{l2,j} = d_{l2} \quad (3)$$

$$\sum_j P_{l2,j} = P_{l2}^{\Sigma} \quad (4)$$

$$d_{l2}^{\min} \leq d_{l2} \leq d_{l2}^{\max} \text{ are integer and } v_{l2,j} \text{ are binary} \quad (5)$$

Type III. Controllable loads over time with a non-interruptible work cycle: These are loads that that once started can not be switched off until the whole fixed-duration work cycle is completed. It is assumed that the load consumption in the unit interval of the work cycle with a fixed duration d_{l3*} is P_{l3*} . Once the work cycle has begun, it can not be interrupted. To ensure this requirement, 3 sets of binary variables are introduced:

$s_{l3,j} = 1$ if the load starts a cycle at the beginning of j

$v_{l3,j} = 1$ if the load is running at power P_{l3*} in the interval j

$f_{l3,j} = 1$ if the load finishes its work cycle at the beginning of the interval j

Because the hour consumption of the load P_{l3*} is a constant additions of the form $v_{l3,j}P_{l3*}$ must be introduced in the balance constraints.

The constraint handling the duration of the work cycle remains unchanged:

$$\sum_j v_{l3,j} = d_{l3*} \quad (6)$$

Constraints ensuring the un-interruptible requirement for the working cycle are introduced:

$$s_{l3,j} - v_{l3,j} \leq 0 \quad (7)$$

$$s_{l3,j} - f_{l3,j} = v_{l3,j} - v_{l3,j-1} \quad (8)$$

$$f_{l3,j} + v_{l3,j} \leq 1 \quad (9)$$

$$s_{l3,j} + \sum_{k=j+1}^{j+d_{l3*}-1} f_{l3,k} \leq 1 \quad (10)$$

Type IV. Controllable loads over time and power level with a non-interruptible work cycle: In this case both the duration $d_{l4}^{\min} \leq d_{l4} \leq d_{l4}^{\max}$ of the work cycle is optimized and the power level at a unit interval $P_{l4}^{\Sigma} / d_{l4}^{\max} \leq P_{l4,j} \leq P_{l4}^{\Sigma} / d_{l4}^{\min}$. Constraints ensuring the un-interruptible requirement for the working cycle must be added using the three sets of binary variables:

$s_{l4,j} = 1$ if the load starts a cycle at the beginning of j

$v_{l4,j} = 1$ if the load is running at power $P_{l4,j}$ in the interval j

$f_{l4,j} = 1$ if the load finishes its work cycle at the beginning of the interval j

In the balance constraints only the power of the load $P_{l4,j}$ is added being and optimization variable. A constraint for the work

cycle duration is present with respect to the simple bounds $d_{l4}^{\min} \leq d_{l4} \leq d_{l4}^{\max}$:

$$\sum_j v_{l4,j} = d_{l4} \quad (11)$$

The following constraints ensure the un-interruptible work cycle and the power levels:

$$s_{l4,j} - v_{l4,j} \leq 0 \quad (12)$$

$$s_{l4,j} - f_{l4,j} = v_{l4,j} - v_{l4,j-1} \quad (13)$$

$$f_{l4,j} + v_{l4,j} \leq 1 \quad (14)$$

$$\sum_j P_{l4,j} = P_{l4}^{\Sigma}, P_{l4,j} - v_{l4,j} P_{l4}^{\max} \leq 0 \text{ and}$$

$$P_{l4,j} - v_{l4,j} P_{l4}^{\min} \geq 0 \quad (15)$$

3. A numerical example

To illustrate the controllable loads with a work cycle modeling techniques the following nomenclature and presumptions might be used. A semi-autonomous building has available controllable and uncontrollable loads and generators and can also purchase or sell power to the external grid. Forecasts for its own uncontrollable load and generation are available as well as prices for buying and selling power.

In the model formulation 'P' stands for 'Power', indices 'n' represent 'non', 'f' stands for 'fixed', 'l' stands for 'load', 'G' stands for 'Generation' and 'a' stands for 'accumulation'. The scenario under consideration includes equal hourly pricing for selling and purchasing power from the network ($c_{buy,t} = c_{sell,t}$) and relatively high price for the own generation units ($c_{nfG} > \max\{c_{buy,t}\}$). The numerical example uses a dataset (given $P_{fG,j}$ and $P_{l,j}$) aiming at maximization of total profit:

$$\max J = \sum c_{sell,j} P_{sell,j} - \sum c_{buy,j} P_{buy,j} - \sum c_{nfG,j} P_{nfG,j} \quad (16)$$

The power of the controllable loads consists of total of seven members divided in four groups of loads according to the classification given in the beginning.

Two loads are from Type I with fixed work cycle duration that can be interrupted and power:

$$d_{l1,1*} = 3 \text{ hours}, P_{l1,1*} = 2,2 \text{ kWh}$$

$$d_{l1,2*} = 4 \text{ hours}, P_{l1,2*} = 2,5 \text{ kWh}$$

Two loads are from Type II with non-fixed power and duration of the work cycle and it can also be interrupted::

$$d_{l2,1} \text{ might be between 2 up to 4 hours, } P_{l2,1}^{\Sigma} = 8,2 \text{ kWh}$$

$$d_{l2,2} \text{ might be between 3 up to 7 hours, } P_{l2,2}^{\Sigma} = 14 \text{ kWh}$$

Two loads from Type III with fixed work cycle duration and power in a unit interval but the continuity of the cycle can not be interrupted:

$$d_{l3,1*} = 2 \text{ hours and } P_{l3,1*} = 1,8 \text{ kWh}$$

$$d_{l3,2*} = 4 \text{ hours and } P_{l3,2*} = 1,4 \text{ kWh}$$

A single load from the last Type IV is considered and its work cycle is un-interruptible. Its work cycle duration is optimized as well as its power in the unit time interval:

$$d_{l4} \text{ may be 3 up to 6 hours with } P_{l4}^{\Sigma} = 12 \text{ kWh}$$

The balance constraint includes all controllable loads additional variables:

$$P_{sell,j} + P_{a,j} + \sum_{l_1=1}^{L_1} v_{l1,j} P_{l1*} + \sum_{l_2=1}^{L_2} P_{l2,j} + \sum_{l_3=1}^{L_3} v_{l3,j} P_{l3*} + \sum_{l_4=1}^{L_4} P_{l4,j} + L_j = P_{buy,j} + P_{R,j} + P_{Ga,j} + P_{G,j} \quad (17)$$

The total power consumed by the controllable loads for the whole optimization period must be not less than the technological minima:

$$\sum_{l_1=1}^{L_1} v_{l1,j} P_{l1*} + \sum_{l_2=1}^{L_2} P_{l2,j} + \sum_{l_3=1}^{L_3} v_{l3,j} P_{l3*} + \sum_{l_4=1}^{L_4} P_{l4,j} \geq E_T \quad (17)$$

For each load the respective additional constraints (1-15) must be added: two constraints of type (2) for each controllable load $l_1 \in L_1$ (Type I), for each controllable load $l_2 \in L_2$ (Type II) a set of constraints (2) to (5), for each controllable load $l_3 \in L_3$ (Type III) a set of constraints (6) to (10) and for the single controllable load $l_4 \in L_4$ (Type IV) the constraints (11) to (15).

Table 1: Optimal values of the variables for accumulation, generation, buying and selling and own controllable generator

Hour j	$P_{a,j}$	$P_{Ga,j}$	$P_{buy,j}$	$P_{sell,j}$	$P_{G,j}$
Col. №	1	2	3	4	5
1	0	0	0	3,3	50
2	0	33,2	33,2	0	0
3	0	31,4	31,4	0	0
4	0	33,9	33,9	0	0
5	0	43,5	43,5	0	0
6	0	39,4	39,4	0	0
7	0	0	0	33,8	0
8	0	0	0	41,2	0
9	10	0	0	51,1	0
10	16	0	0	71	0
11	16	0	0	60	0
12	16	0	0	54,7	0
13	16	0	0	66	0
14	0	0	0	58	0
15	0	0	0	39,1	0
16	0	0	0	76,6	0
17	0	0	0	59,2	0
18	16	0	0	53,5	0
19	16	0	0	37,2	0
20	16	0	0	6,3	0
21	16	0	0	8	0
22	16	0	0	8	0
23	0	28	28	0	0
24	0	28	28	0	0

The constraint (19) stands for the accumulation-generation efficiency coefficient η . The fact that no purchasing and selling in a time interval is allowed, as well as accumulation and generation from accumulating units is not possible two sets of binary variables are introduced in the model ($v_j = 1$ when buying power from the external network and $u_j = 1$ when generating power from the accumulation units) to construct the mutually exclusive alternatives. Constraints (20) assure that no purchase and selling power onto the external grid will occur in a same time interval. Constraints (21) assure that no accumulation and generation will occur in a same time interval. The power of the controllable generator is fixed above (22).

$$\eta \sum P_{a,j} = \sum P_{Ga,j} \quad (19)$$

$$P_{sell,j} \leq (1 - v_j) P_{sell}^{\max} \quad \text{and} \quad P_{buy,j} \leq v_j P_{buy}^{\max} \quad (20)$$

$$P_{a,j} \leq (1 - u_j) P_a^{\max} \quad \text{and} \quad P_{Ga,j} \leq u_j P_{Ga}^{\max} \quad (21)$$

$$P_{nfG,j} \leq P_{nfG}^{\max} \quad (22)$$

The optimal values of the variables are given in Tables 1 and 2. The optimal working cycle durations for the loads of Groups II and

IV loads are 2 hours, 3 hours and 6 hours respectively. Since best prices are night, all controllable loads under consideration work at night (Table 2). With such levels of the fixed generation the building can not function autonomously, i.e. without buying and selling from the external grid, because the sum load from the controllables (18.7 kWh) and the maximum possible P_a^{Max} value can not equal the estimated difference between fixed generation and load (76.6 kWh at 16h).

Table 2: Optimal values for the controllable loads consumption over the optimization horizon

j №	$P_{1,1,j}$ 1	$P_{1,2,j}$ 2	$P_{1,3,j}$ 3	$P_{1,4,j}$ 4	$P_{2,1,j}$ 5	$P_{2,2,j}$ 6	$P_{3,1,j}$ 7
1	2,2	2,5	4,1	4,7	1,8	1,4	2
2	0	0	0	0	1,8	1,4	2
3	0	0	0	0	0	1,4	2
4	0	2,5	0	0	0	1,4	2
5	2,2	2,5	4,1	4,7	0	0	2
6	2,2	2,5	0	4,7	0	0	2
7	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0
13	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0
18	0	0	0	0	0	0	0
19	0	0	0	0	0	0	0
20	0	0	0	0	0	0	0
21	0	0	0	0	0	0	0
22	0	0	0	0	0	0	0
23	0	0	0	0	0	0	0
24	0	0	0	0	0	0	0

This building can operate in a mode without buying from the external network ($P_{buy,j} = 0$) but just selling ($0 \leq P_{sell,j}$). With such a realization of the building's operation, the optimal timetable for the operation of the controllable loads shifts to the afternoon hours (Tables 3 and 4).

Table 3: Optimal values of the variables for accumulation, generation, buying and selling and own controllable generator when only selling is allowed

Hour j Col. №	$P_{a,j}$ 1	$P_{Ga,j}$ 2	$P_{buy,j}$ 3	$P_{sell,j}$ 4	$P_{G,j}$ 5
1	20	0	0	8,5	50
2	0	8	0	0	0
3	0	8	0	0	0
4	0	8	0	0	0
5	0	8	0	0	0
6	0	8	0	0	0
7	20	0	0	14,5	0
8	20	0	0	26,0	0
9	20	0	0	17,1	0
10	0	0	0	55	0
11	0	0	0	44	0
12	0	0	0	38,7	0
13	0	0	0	50	0
14	20	0	0	36,6	0
15	20	0	0	35,2	0
16	20	0	0	55,2	0
17	20	0	0	37,8	0
18	0	0	0	37,5	0
19	0	16	0	37,2	0
20	0	16	0	6,3	0
21	0	16	0	8	0
22	0	8	0	0	0
23	0	8	0	0	0
24	0	8	0	0	0

The accumulation and generations schedule changes as well as the optimal duration of the single load from the fourth group (L4) as it becomes 3 hours.

Table 4: Optimal values for the controllable loads consumption over the optimization horizon when only selling is allowed

j №	$P_{1,1,j}$ 1	$P_{1,2,j}$ 2	$P_{1,3,j}$ 3	$P_{1,4,j}$ 4	$P_{2,1,j}$ 5	$P_{2,2,j}$ 6	$P_{3,1,j}$ 7
1	2,2	2,5	4,1	4,7	0	0	0
2	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0
7	2,2	2,5	4,1	4,7	1,8	0	4
8	2,2	2,5	0	4,7	1,8	0	4
9	0	0	0	0	0	0	4
10	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0
13	0	0	0	0	0	0	0
14	0	0	0	0	0	1,4	0
15	0	2,5	0	0	0	1,4	0
16	0	0	0	0	0	1,4	0
17	0	0	0	0	0	1,4	0
18	0	0	0	0	0	0	0
19	0	0	0	0	0	0	0
20	0	0	0	0	0	0	0
21	0	0	0	0	0	0	0
22	0	0	0	0	0	0	0
23	0	0	0	0	0	0	0
24	0	0	0	0	0	0	0

4. Conclusion

An approach to controllable loads with a working cycle consisting of more than one unit interval is proposed. The same modeling technique is used for power generating units start-up and stopping cycles in problems for optimal thermal units maintenance medium-term planning. The latter is a modification of the unit commitment problem but its result influence the UC solution as availability. The numerical example shows how binary and integer values handle the physical requirements of the controllable loads. It also shows the sensitivity towards simple bounds over one set of optimization variables and its interpretation.

5. Bibliography

- [1] Saravanan, B., Das, S., Sikri, S. et al., A solution to the unit commitment problem - a review, *Frontiers in Energy* (2013) Vol 7: pp. 223-226, <https://doi.org/10.1007/s11708-013-0240-3>
- [2] Стоилов Д. Г., Янев К. И., Избор на състава на работещите агрегати в електроенергийните системи чрез смесено-целочислено линейно програмиране, списание *Енергетика*, брой 5, 2000 г., стр 21-23
- [3] Стоилов Д., Ваковски Д., Алгоритми за оптимално разместване на планираните престои на агрегатите от КЕЦ в условия на дефицит, *Енергиен форум'2007*, Варна, юни 2007г., Сборник доклади том II, стр. 221-226.
- [4] Стоилов Д., Кънева М., Ваковски Д., Математически модел за оптимално разпределяне на планираните престои на кондензационните агрегати в условия на дефицит, *Списание Енергетика*, брой 6, 2007г.
- [5] 122 Viana A., Pedroso J. P., A new MILP-based approach for Unit Commitment in power production planning, *International Journal of Electrical Power & Energy Systems*, Volume 44, Issue 1, January 2013, p. 997-1005

NUMERICAL MODEL FOR SIMULATION OF THE VELOCITY FIELDS FOR THE EXPLOSIVELY FORMED PENETRATOR

ЧИСЛЕН МОДЕЛ ЗА СИМУЛАЦИЯ НА СКОРОСТНИТЕ ЗОНИ ПРИ ЗАРЯДИ ОТ УДАРНО ЯДРО

M.Sc. Hutov I. PhD.¹, Prof. M.Sc. Lilov I. PhD.²

Joint Forces Command – Sofia, Bulgaria¹

“Vasil Levski” National Military University, Veliko Turnovo, Bulgaria²

i.hutov@armf.bg

Abstract: The current paper presents numerical approach of velocity performances estimations for the EFP (Explosively Formed Projectiles). The proposed method mathematically develops velocities parameters of a particular segment for EFP liner propelled by explosive process. The numerical method is developed, to provide estimations about behavior of projectile vs. time in the EFP forming process powered by explosion. The model is valid for performances estimations of EFP warheads and design data for optimal EFP configuration. Simulations are supported by the software Autodyn for numerical modeling respectively. The obtained numerical results are compared with the available experimental data.

KEYWORDS: EXPLOSIVE FORMED PENETRATOR, NUMERICAL SIMULATION, VELOCITIES DISTRIBUTION, AUTODYN,

1. Introduction

Nowadays, the EFP warheads are present in many systems that expect appropriate modernization and/or optimization; as artillery sub-munitions, antitank missiles, mines etc. Approaches which define the processes of explosively formed projectiles [1-4] are one of the most sophisticated problems of rigid body mechanics based on the elastic to plastic theory. The distinguishing problem of the EFP projectiles is the velocity of the EFP liner. This velocity is generated in the explosively driven process and the dynamics of their evolution is the main topic of this paper. Recently, most papers are based on numerical methods [5-10] which determine the projectiles velocity performances based on detailed modeling of the loadings and deformation process during explosion. Numerical software, particularly Autodyn, which is often used for detailed analyses in numerical simulations, require comprehensive preparation of the expected initial data but some others methods as it analytical are less precise but enough reliable and provides much faster data obtaining for the applications of warheads performances estimations.

The current paper presents software based on the previously studied analytical method as a solution to provide the ability to preliminarily estimations as well as numerical solution of the same rooted liners velocities. This methodology provides ability to analyze the adopted design of warhead's performances by more precise numerical software like Autodyn.

The research based on the analytical models presented in papers [1-5], provides crucial information about the EFP performances in a short time without required comprehensive initial data preparation. The algorithm presented in further papers provides the possibility to directly export the adopted geometry of EFP liners integrated with warheads into Autodyn numerical software, from the software package Matlab, which considerably decreases preparation time.

The results of numerical method contribute in improving the accuracy of EFP velocity estimations. This is achieved by an appropriate augmentation in the number of the grid elements for the method used.

2. Numerical approach

Numerical approach based on the finite element method is used in this research in order to be compared with experimental data.

The properties of the adopted simulation model mesh [12-19] are given in Table 1. The mesh density is determined taking into account accuracy as well as reasonable simulation run time within available computer facilities.

Figure 1a and 1b shows configuration of EFP warhead as well as appearance of created mesh for each component separately.

The simulation sample volume in numerical approach is observed as the quarter shown on the figure 1a and 1b.

Presented analysis uses fully Lagrangian solver, where after 35 μ s, detonation products are not influenced into forming processes. But that average liners final velocity comparative with analytical modeling corresponds not to the 35 μ s instant of forming time then about 70-150 μ s where dynamical process is fully completed (figures 5 and 6).

A wide range of metal powders (from light alloys through steels to super-alloys and composites) is currently available for DMLS process and other new materials are under development. Table 1 lists mechanical properties of selected powder materials.

Table 1: Grid properties of the numerical approach [3]

Conditions	Type 1		Type 2*	
	1	2	1	
Liner	7776	6125	7776	6125
Explosive	10496	9000	10496	9000
Cover	15006	12000	-	-
Back plate	768	450	768	450
1 – nodes; 2 –elements;				

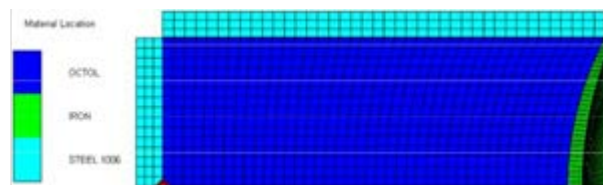


Figure 1a: Geometrical configuration of EFP sample type1 (with cover) and finite elements mesh

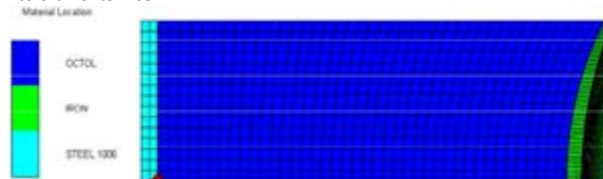


Figure 1b: Geometrical configuration of EFP sample type2 (without cover) and finite elements mesh

The loading forces distribution model is expressed by the detonation pressure products and is determined according to Jones-Wilkins-Lee [1] by the equation of state:

$$p = K \left(1 - \frac{\omega}{R_1 V} \right) e^{(-R_1 V)} + K_1 \left(1 - \frac{\omega}{R_2 V} \right) e^{(-R_2 V)} + \frac{\omega E}{V} \quad (1)$$

where V and E are represented as $V = \rho_0/\rho$, $E = \rho_0 e$, ρ_0 is the current density, ρ is the reference density, e is the specific internal energy and K, K_1, R_1, R_2 and ω are constants for the given explosive material [1,2].

3. Simulation model

The comparison of these methods is performed on the sample design fig 2, with accepted, fixed EFP liner form and explosive charge, with and without metal cover. Adopted explosively driven projectile model and its elements of geometry, presented in the paper [2], and design characteristics of testing sample as in the [14] are shown in Fig. 2. The model does not include the fuze and wave shaper integrated in the warhead design and influenced on the real performances modeling.

The properties of explosive and other materials used in simulations are given in Table 1 [14]. In tested examples, the initiation point is located on the warhead bottom and lies on axis of symmetry [14] (Fig. 1).

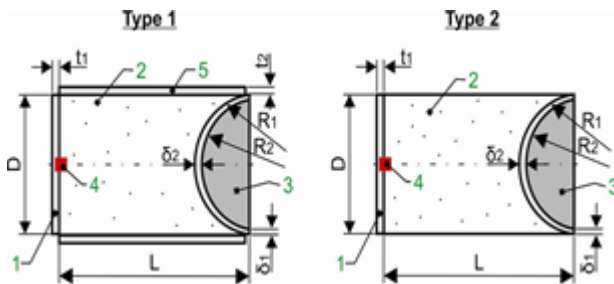


Figure 2: Types of testing sample and their basic dimensions: 1-back plate, 2-explosive charge, 3-liner, 4-initiation point, 5-cover.

Table 2: Geometrical parameters for EFP sample models [3]

Design parameter		Type 1	Type 2*
Length of charge	L [mm]	85	85
Caliber	D [mm]	57.2	57.2
Thickness of back plate	t1 [mm]	5	3
Cover thickness	t2 [mm]	5	-
Inner radius	R1 [mm]	60.4	71.3
Outer radius	R2 [mm]	60.4	71.3
Thickness of liner edge	delta1 [mm]	1.5	1.5
Thickness of liner center	delta2 [mm]	2.7	2.7
Type initiation		p.	p.
* -experiment; p. -point initiation			

Analytical and numerical approach used Octol as explosive material with density of 1.82 g/cm³ and detonation velocity 8480 m/s as well as steel as cover and iron as liner material. The experimental sample was tested on the proving ground as a type 2 [14] in Table 2.

4. Results and discussion

Two types of simulation samples of the liners and explosives

integrated have been considered through represented modeling in numerical approach.

Figures 3 and 4 show energy distribution vs. time during projectile forming. Kinetic energy represents penetration capability of formed projectiles.

The plastic works, is important for liners' design and for selection of appropriate material. Figure 3 and 4 represents nonlinear and uniform distribution of plastic energy. It means that liner during formation had proper deformation also influenced on the velocities distribution. If that curve in initial phase of formation has no permanent increase, this indicates the liner had the fracture.

Table 3 shows differences in the energy distribution obtained by the numerical and analytical approach. In table 3 are presented next values: absolute initial velocity V_0 [m/s], kinetic energy E_k [J], axial deformation energy ADE [J], radial deformation energy RDE [J] and plastic deformation energy/plastic work PW [J].

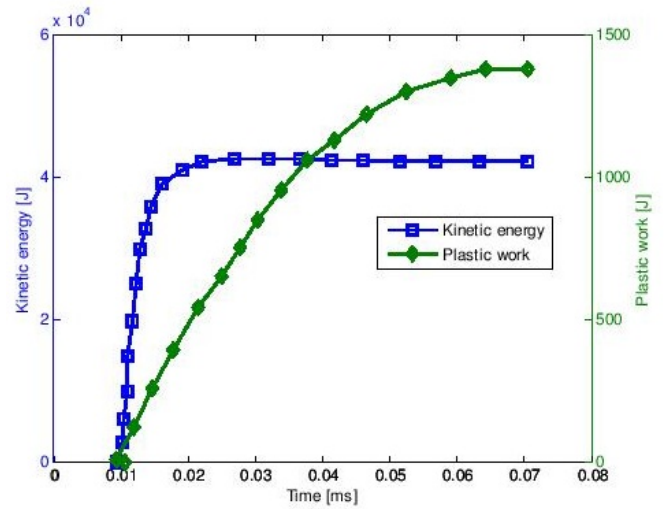


Figure 3: Energy distribution during time of the forming of explosively formed projectile, sample type 1, obtained by numerical method [3]

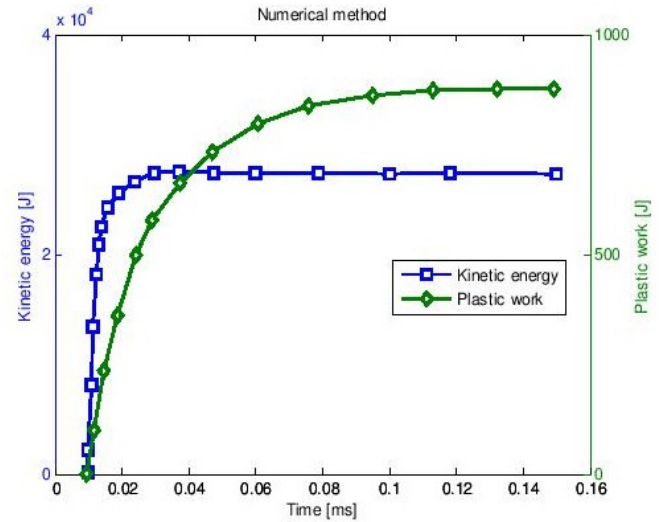


Figure 4: Energy distribution during time of the forming of explosively formed projectile, sample-type 2, obtained by numerical method [3]

These parameters are collected as the consequence of considering problems of deformation energy in the numerical and in the analytical models. Differences between two types of samples show that cover of the explosive sample influences as to increase of kinetic energy of projectile and also the increase of total plastic deformation work [1,2,10,13,20].

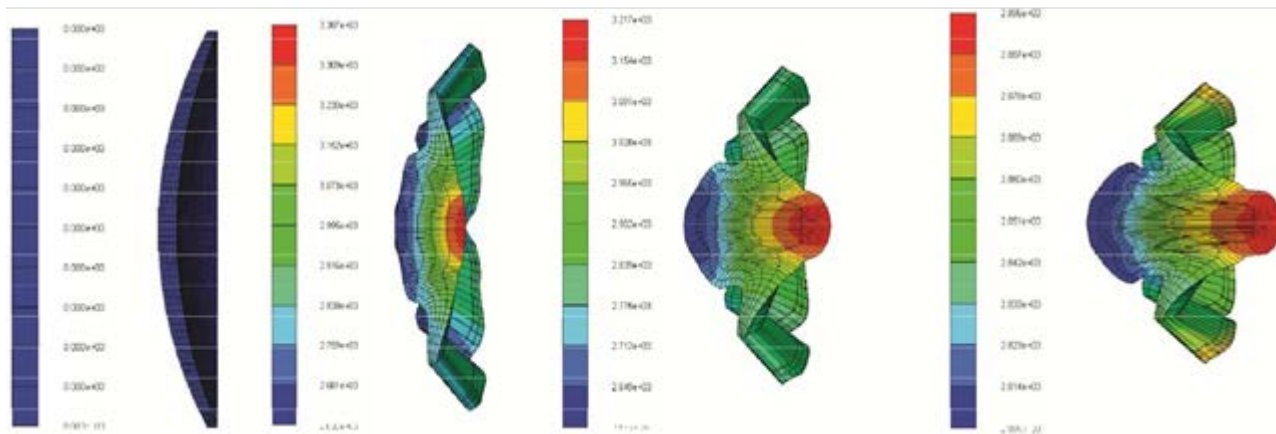


Figure 5: Shape of projectile configuration during forming to the final shape in 70 μ s of sample-type 1

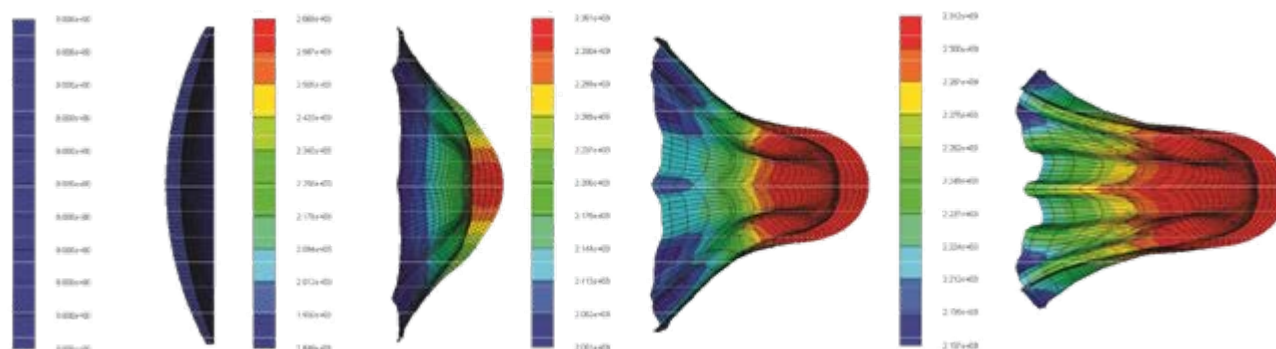


Figure 6: Shape of projectile configuration during forming to the final shape in 150 μ s of sample-type 2

Numerical simulation also reproduces expected shapes of projectiles at the end of forming process shown in (Figs. 5 and 6). For the sample type 1 (Fig. 5) projectile is formed with its final shape after $t=70.5 \mu$ s at the distance 265.31mm, realizing final velocity of about 2860 m/s. For the sample type 2 (Fig. 6) these values are corresponding to the instant $t=150 \mu$ s, at the distance 418.2 mm and velocity 2435 m/s. That means that sample type 2 has much less coefficient of energy efficiency than covered warhead charges [10]. The final projectile shape joint with considered velocity performances influences two basic performances important for EFP warhead design – penetrability and precision.

5. Conclusion

The next conclusions are presented as the result of this study:

The numerical approach is a well-designed tool for the EFP velocity and energy modeling and estimations.

Numerical method gives more accurate results regarding velocity in comparison with analytical methods and these results are very close to experimental data, with error of less than 1.5%. It should be noted that numerical method is useful for the shortening the development time of EFP warheads during design and reduces the cost of their experimental testing.

The same configuration of liners and explosive charges with and without metal covers produced different shapes of explosively formed projectiles. Sample type 1 produced EFP as the plastic solid shape less adoptable for distance flight, and sample type 2 produced EFP with more adoptable shape for distance flight regarding aerodynamical drag.

6. Literature

- [1] Орленко, Л.П. : *Физика Взрыва*, Главная редакция физико-математической литературы, Москва, 2004.
- [2] Sharma, VK, Kishore, P., Bhattacharyya, AR, Raychaudhuri, TK, Singh S.: *An Analytical Approach for Modeling EFP Formation and Estimation of Confinement on Velocity*, International Ballistics Society, pp.565-574.
- [3] Marković, M., Elek, P., Jaramaz, S. Milinović, M., Micković, D.. “Numerical and analytical approach to the modeling of explosively formed projectiles”, 6th International Scientific Conference OTEH 2014, October Belgrade, pp. 9-10, 2014.
- [4] Marković, M.: *Explosively Formed Projectiles*, MSc Thesis, University in Belgrade, Mechanical Engineering, Weapon Systems Department, 2011.
- [5] Markovic, M., Milinovic, M., Elek, P., Jaramaz, S., Mickovic, D. “Comparative approaches to the modeling of explosively formed projectiles”, Proceedings of Tomsk State University, Serie Physics and Mathematics, V.293, 2014.
- [6] Markovic M., Milinovic M., Jeremic O., Jaramaz S.. “Numerical modeling of temperature field on high velocity explosively formed projectile”, 17th Symposium On Thermal Science And Engineering Of Serbia, October 20–23, pp.175-181, 2015.
- [7] Pappu, S., Murr, L.E.: *Hydrocode and microstructural analysis of explosively formed penetrators*, Journal of Materials Science, pp. 233-248, 2002.
- [8] Hussain, G., et al.: *Gradient Valued Profiles and L/D Ratio of Al EFP With Modified Johnson Cook Model*, Journal of Materials Science and Engineering 5, pp. 599-604, 2011.
- [9] Fedorov, S.V., Bayanova Ya. M., Ladov, S.V. “Numerical analysis of the effect of the geometric parameters of a combined shaped-charge liner on the mass and velocity of explosively formed

compact elements”, Combustion, Explosion, and Shock Wave, Vol. 51, No. 1, pp. 130-142, 2015.

[10] Hussain, G., Hameed, A., Hetherington, J.G. “Analytical performance study of explosively formed projectile”, Journal of applied mechanics and technical physics, Vol.54, No.1, pp.10-20, 2013.

[11] Bender, D., Corleone, J. “*Tactical Missile Warheads - Explosively Formed Projectile*”, American Institute of Aeronautic and Astronautic, Washington, 1993.

[12] Teng, T.L., Chu, Y.A., Chang, f.a., Shen, B.C. “*Design and Implementation of a High Velocity Projectile Generator*”, Fizika Goreniya i Vzryva, Vol. 43, No. 2, pp. 233-240, 2007.

[13] Weimann, K. “Research and development in the area of explosively formed projectiles charge technology”, Properllants, Explosives, Pyro-technics, Vol. 18, pp. 294-298, 1993.

[14] Jones, D.A., Kemister, G., Borg, R.A.J.: *Numerical Simulation of Detonation in Condensed Phase Explosives*, Weapons Systems Division Aeronautical and Maritime Research Laboratory, August 1998.

[15] Lam, C., McQueen, D.: *Study of the Penetration of Water by an Explosively Formed Projectile*, Weapons Systems Division Aeronautical and Maritime Research Laboratory, June 1998.

[16] Fong, R., Kraft, J., Thompson, L.M., Ng, W.: *3D Hydrocode Analysis of Novel Asymmetrical Warhead Designs*, Proceedings for the Army Science Conference (24th), 29 November - 2 December, Florida, pp.1-3, 2005.

[17] Weibing, L., Xiaoming, W., Wenbin, L.: *The Effect of Annular multi-point Initiation on the Formation and Penetration of an Explosively Formed Penetrator*, International Journal of Impact Engineering 37, pp. 414-424, 2010.

[18] Church, P.D., Cullis, I.: *Development and Application of High Strain Rate Constitutive Models in Hydrocodes*, Journal de Physique IV, Vol. 1, pp. 917-922, October 1991.

[19] Luttwak, G., Cowler, M.S.: *Advanced Eulerian Techniques for the Numerical Simulation of Impact and Penetration using AUTODYN-3D*, International Symposium of Interaction of the Effects of Munitions with structures, Berlin, 3-7 May, 1999.

[20] Jianfeng, L., Tao, H., Longhe, L., Bing, H.: *Numerical Simulation of Formation of EFP With Charge of Aluminized High Explosive*, International Symposium on Ballistics, Tarragona, Spain 16-20 April, 2007.

MODELING OF PRODUCTION PARAMETERS OF B₄C + ZrO₂ COMPOSITES VIA ARTIFICIAL NEURAL NETWORKS METHOD

S. Hartomacıoğlu. PhD.¹, H.O.Gülsoy. PhD.², B. Bakırcıoğlu Ms.C.³
Department of Mechanical Engineering – Marmara University, Turkey¹
Department of Metallurgy and Materials Engineering– Marmara University, Turkey²
Department of Mechatronics, Selcuk University, Turkey³
selimh@marmara.edu.tr

Abstract: In this study, the effect of production parameters of B₄C + ZrO₂ composites on density was modelled by using Artificial Neural Network (ANN). The composites were produced by using powder injection molding method (PIM). In the sintering stage, pressureless sintering method under argon atmosphere was used. As the production parameters, amount of additional (A, wt.%) and sintering temperature (T, °C) were defined. The main aim of the study is to obtain the experimental conditions giving maximum density. As a results of this study, the production parameters of hard sintered materials like B₄C + ZrO₂ could be modelled by using ANN method to optimize and predict because the prediction error is blow percentage of 10%. Therefore, the research and development time and cost can be reduced by using this method.

Keywords: POWDER INJECTION MOLDING, ARTIFICIAL NEURAL NETWORK, MODELING

1. Introduction

In the literature, most of article about sintering of boron carbide is related to fabrication of boron carbide via hot isostatic pressing and hot pressing method. There are several studies in the literature about the pressureless sintering of boron carbide with additive or non-additive. T.K. Roy et al produced boron carbide ceramics with and without additives (C, TiB₂, and ZrO₂) by pressureless sintering method to obtain dense samples for use as neutron absorber in fast breeder reactors in 2006. They investigated the effect of particle size and sintering temperature on density and microstructure. The compacts were fired in the temperature range of 2225-2375 °C under vacuum [1]. The effect of ZrO₂-3 % Y₂O₃ addition on densification, sintering behavior and mechanical properties of B₄C was studied by H.R. Baharvandi et al in 2006. The adding amount of ZrO₂-3 % Y₂O₃ was 0-30 wt.% and sintering temperature was between 2050-2150 °C [2]. In the 2007, the B₄C-metal boride composites were derived from B₄C/metal oxide mixture by A. Goldstein et al. The green pellets were sintered from room temperature to 2180 °C under Ar atmosphere via pressureless sintering method. In this study, TiO₂, ZrO₂, V₂O₅, Zr₂O₃, Y₂O₃ and LaO₃ were used for addition [3].

In this study, B₄C + ZrO₂ composites based part produced by powder injection molding method were investigated Density properties of the sintered products were evaluated in sintered condition. The production parameters were modelled using artificial neural network method.

2. Materials and Method

Materials

Boron Carbide (B₄C) is an important non-metallic hard material with high melting point (2450 °C), high hardness (25 to 35 GPa- next only to diamond and cubic boron nitride), high elastic modulus (450 GPa), high flexural strength (350-500 MPa) and low density (2.52 g/cm³) [1, 4]. ZrO₂ is the ceramic material with adequate mechanical properties. In this thesis study, commercially available B₄C powder (ABSCO Co, UK) was used. Additive powder, ZrO₂ Stack, Germany) powders were used. For molding the mixing powders, binder materials and their rates must be defined. The primary required the binder is to allow flow of the particles into the cavity. Paraffin Wax (PW), Carnauba Wax (CW), Polypropylene (PP) and Stearic Acid (SA) were selected for binder system.

Some properties of binder system components are shown in Table 1.

Table 1: Some properties of the binder system components

Binder Type	Density (g/cm ³)	Melting Point °C
Paraffin Wax (MERC)	0.9	90
Carnauba Wax (MERC)	0.97	112
Polypropylene (MERC)	0.89	161
Stearic Acid (MERC)	0.85	73

Method

Powder Injection Molding (PIM) which enables to produce products with high dimensional accuracy in such a way to have excellent, fine grain structure and non-anisotropic mechanical properties [5] is an advanced manufacturing technology. The other words, PIM method is a new technology and uses the shaping advantage of injection molding but it is applicable to metals and ceramics. Complex, precision, and net shape components are produced by PIM method from metal or ceramic powder. In recent years, PIM has established it-self as a cost-effective production technique derived from plastic injection molding, allowing large scale production of complex part [6]. The product produced by PIM is expected to have more homogenous microstructure since hydraulic pressure is filled up uniformly. Also. Fabrication cost could be eliminated significantly by reducing machining and recycling use of feedstock [7].

PIM method has four steps: 1) Preparation of feedstock, 2) Injection of molding, 3) Solvent and thermal debinding, 4) Sintering [8, 9]. The flow chart of PIM method is shown in Figure 1.

The first mold was designed based on Metal Powder Industries Federation (MPIF) standard 50. The mold was shown in Figure 2.

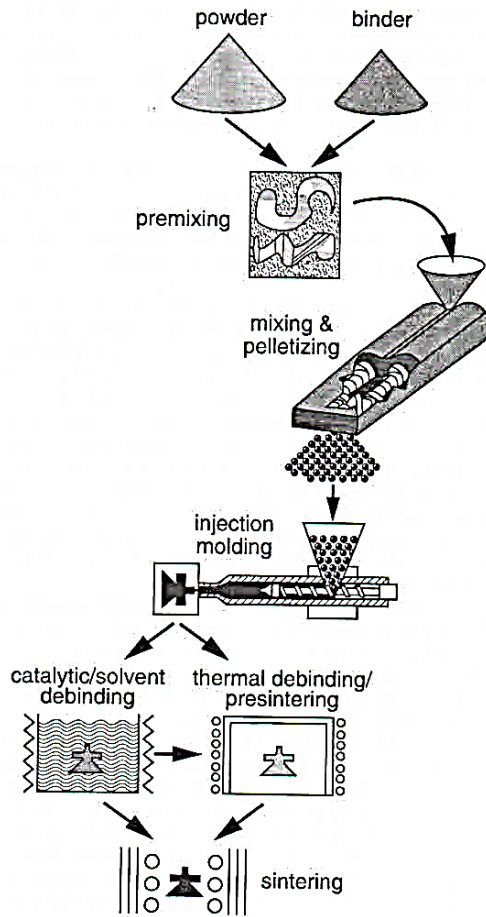


Figure 2 Flow chart of powder injection molding method [7]

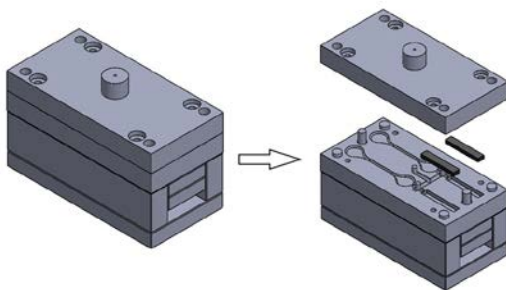


Figure 3 The mold based on MPIF 50 and 59 standard

As a results of pre-experimental studies of PIM methods, the optimal binder materials ratio was defined and listed in Table 2.

Table 2 Mixture ratio of binder system

Binder Types	PW (wt. %)	CW (wt. %)	PP (wt. %)	SA (wt. %)
Mixture Ratio	69	10	20	1

The full factorial experimental design was used as preparation experimental table. The Input parameters and their levels of experimental design was shown in Table 3.

Factors	1	2	3	4	5	6
A: Amount of Ad. (wt.%)	0	2	4	8	12	16
B: Sint. Temp.(°C)	2000	2100	2200			

The total experimental number according to full factorial experimental design is 18 experiments. The experiment conditions of each experiment number was prepared. The main powder and additive powder was mixed using Turbula Mixer with 3 dimensional motion to be obtained homogenous mixing. The next step, the feedstock was prepared for powder injection molding procedure. In this step, special custom made device was used. The mixed powder and binder system materials was mixed under 130 °C temperature and 200 rev./min mixing speed. The granules were obtained by hand and the standard samples were injected by custom made powder injection molding device. In the injection molding device, molding pressure was 15 bar, clapping pressure 10 bar, barrel temperature was 160 °C, and Molding speed was 15 sec. From the injected parts, the binder other than Polypropylene was achieved debinding in solvent. In this step, to provide uniform temperature, hot water was circulated continuously around the container of samples with heptane. Thermal debinding process was performed in furnace under Ar atmosphere. After the debinding processes, the samples were sintered using custom made sintering furnace with graphite resistance under Ar atmosphere.

After the sintering, the samples were cut by means of diamond cutting disc. The density of each part was measured by Archimedes Method.

Artificial Neural Network

After the experimental studies, the experimental numerical results were obtained. In the ANN processes, first step the data was normalized between 0 and 1. Then, the data was divided into training data set (75%) and testing data set (25%). After this step, the ANN topology was prepared. In this study, multilayer perceptron (MLP) of ANN structure was used. In this structure, there are three layers: input layer, hidden layer and output layer. In the input layer, the number of processes element (artificial neuron) corresponds to the input parameters of experiments. The output layer processes elements correspond to the output parameters of experiments. In this study, there are 3 artificial neurons in input layer, and there are 1 artificial neuron in output layer. The number of hidden layer neurons was found to be between 1 and 50 by trial and error method under 50 000 epochs. In this study, there are 3 step of ANN procedure, 1) training, 2) testing, and 3) production step. In the training step, optimal ANN structure was obtained using mean square error (MSE) performance criterion. The next step, testing step, the test performance of optimal ANN structure was tested and evaluated. Final step of ANN procedure, the new experimental results were predicted using this optimal ANN structure. The ANN structure of this study was shown in Figure 4.

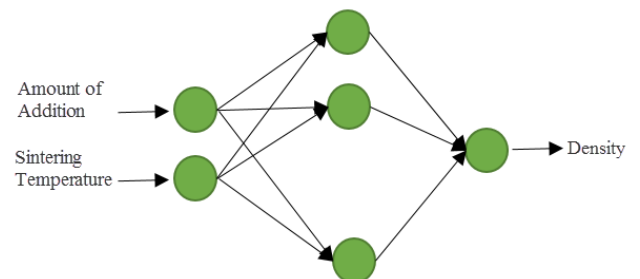


Figure 4 The ANN structure of this study

3. Results and Discussion

After the experimental studies, the experimental results were obtained and the relative density was calculated for each experimental conditions. The experimental results were listed in Table 3.

Table 3 The experimental results

#	A [wt. %]	B [°C]	Y1[%]
1	0	2000	58
2	0	2100	63
3	0	2200	68
4	2	2000	61
5	2	2100	95
6	2	2200	85
7	4	2000	57
8	4	2100	96
9	4	2200	73
10	8	2000	69
11	8	2100	72
12	8	2200	75
13	12	2000	66
14	12	2100	73
15	12	2200	72
16	16	2000	64
17	16	2100	67
18	16	2200	71

After the applying ANN procedure, the training results was shown in Figure 5. The optimal ANN structure was define using this results. In the optimal ANN structure, the number of hidden layer neurons is 20. This value was obtained at 50 000 iterations. Final MSE is 0.46.

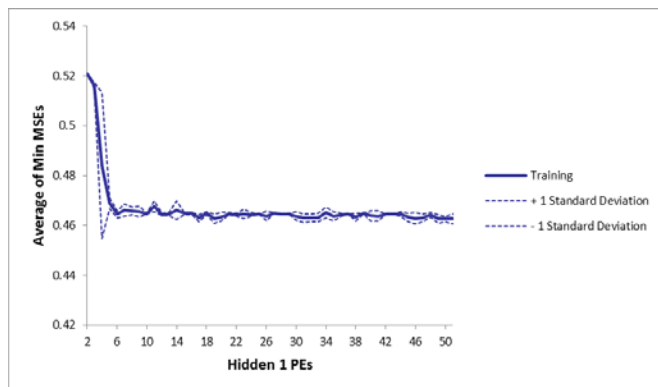


Figure 5: Training results of ANN

In the test steps, the optimal ANN was evaluated by two methods. In the first method, the testing operations was conducted by using training data set, the second method, the testing operations was performed by using test data set. The training data set testing results was shown in Figure 6. In this operations, the correlation coefficient is 0.99, and the percentage error is 0.028%.

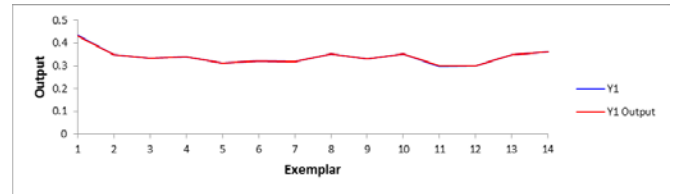


Figure 6 results of training data set testing

The second test operations results were shown in Figure. In this step, the percentage error is %9.36, and correlation coefficient is 0.95.

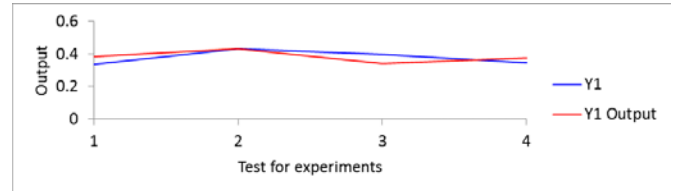


Figure 7 Results of testing data set testing

4. Conclusion

In this study, the production parameters of boron carbide composites were studied and evaluated. Firstly, the powder injection molding method was applied. In this step, the main powder and additive powder was mixed, and then the feedstock was prepared using binder systems. After the granulation, the standard samples were injected. The solvent debinding and thermal debinding processes was applied and then the debinded parts were sintered using different sintering temperature. The densities of sintered samples were measured by using Archimedes Methods, and the theoretical density and relative density values were calculated related formula. After the experimental studies, the optimal ANN structure was obtained using training, and testing operations. In the testing steps, the percentage error of training data set was 0.029%, and correlation coefficient 0.99, the percentage error of testing data set was 9.36% and correlation coefficient is 0.95. The optimal ANN stricter consist three layer; 1) input layer (3 artificial neurons), 2) hidden layer (20 artificial neurons), and 3) output layers (1 artificial neurons). As a results of this study, the artificial neural networks method was used to modeling the production parameters of hard sintered materials like boron carbide composites.

5. Acknowledgements

This work is support by Scientific Research Project Program of Marmara University (Grand: **FEN-K-110117-0019**).

6. References

- [1] Roy, T.K., Subramanian, C., Suri, A.K. (2006) Pressureless Sintering of Boron Carbide. *Ceramic International*, 32, 227-233
- [2] Baharvandi, H.R., Hadian, A.M., Abdizadeh, A. (2006) Investigation on Addition of ZrO₃-3 mol% Y₂O₃ Powder on Sintering Behaviour and Mechanical Properties of B₄C. *Journal of Materials Science*, 41(16), 5269-5272
- [3] Goldstain, A., Yeshurun, Y., Goldenberg, A. (2007) B₄C/Metal Boride Composites Derived from B₄C/Metal Oxide Mixtures. *Journal of the European Ceramic Society*, 27, 695-700
- [4] Beaudet, T.D., Smith, J.R., Adams, J.W. (2015) Surface energy and relaxation in boron carbide (1011) from first principles. *Solid State Communications*, 219, 42-47
- [5] Gülsoy, H.Ö., Özgün, Ö., Bilketaş, S. (2016) Powder injection molding of Stellite 6 powder: sintering, microstructural and mechanical properties. *Material Science & Engineering A*, 651, 914-924

[6] Bleyan, D., Hausnerova, B., Svoboda, P. (2015) the development of powder injection molding binders: A quantification of individual interactions. *Powder Technology*, 286, 84-89

[7] German, R.M. (1996) *Sintering Theory and Practice*, Wiley, San Diego

[8] Baojun, Z., Xuanhui, Q., Ying, T. (2002) Powder injection molding of WC-8%Co tungsten cemented carbide. *International Journal of Refractory Metals & Hard Materials*, 20, 389-394

[9] Nyberg, E., Miller, M., Simmons, K., Weil, K., S. (2005) Microstructure and mechanical properties of titanium components fabricated by a new powder injection molding technique. *Materials Science and Engineering C*, 25, 336-342

GENERATION OF AN ATLAS-BASED FINITE ELEMENT MODEL OF THE HEART FOR CARDIAC SIMULATION

M.Sc. Vasiliev Evgeny
Lobachevsky State University of Nizhny Novgorod, Nizhny Novgorod, Russia
eugene.unn@gmail.com

Abstract: In this paper an algorithm for creating an atlas-based finite element heart model for cardiac simulation is described. This model is used to simulate the propagation of electrical impulses of the heart. An important feature of this model is that it contains conductive paths and fibrous tissue, which makes it possible to make more realistic calculations of the propagation of electrical signals. The model created from anatomical segments of the heart surface is defined by a polygonal mesh. The algorithm presented in the article offers a means to create models of various accuracy.

Keywords: HEART MODEL, CARDIAC SYSTEM, RECONSTRUCTION, RAY CASTING, FE-MODEL, TETRAHEDRAL MESH.

1. Introduction

In order to simulate an accurate electrical system of the human heart, it is necessary to have a detailed heart model containing different types of tissues: the direction of the muscle tissue, conducting fibers, fibrous rings, etc.

Nowadays there is a number of finite element models (FE models) of heart for modeling electricity signals. For example, in some systems of heart electrical modeling, the rabbit heart model is used [R. Bordasa, 2011] [Arevalo HJ, 2016]. The rabbit heart model was constructed from a high resolution MRI dataset, with the use of an intensity based level-set filter.

The first developed 3D models of cardiac anatomy were simplistic models based on geometric shapes, this approach is still in use for applications where the anatomical validity is not important for the purpose of the model [Colli Franzone P, 1998] [Sermesant M, 2006]. Currently, researches use simple geometric shapes and make parameterized models based on segmented heart images [P. Lamata et al, 2014].

In many articles, studies are based on models built on the segmentation of CT [Deng D, 2012] [Aslanidi OV, 2013] or MRI [Plotkowiak M, 2008] [Lopez-Perez & Sebastian, 2015] scans. Models of this type very anatomically accurate, but usually they describe only one heartbeat phase, rather than the whole cycle.

Our algorithm enables automatic marking of vertex the type of tissues after the grid generation, because manual marking of hundreds of thousands and more tetrahedrons makes no sense.

2. Source data

As the initial data, anatomical segments of heart surface from Plastic boy anatomy (Plastic boy store) were used. We have several types of meshes (Figure 1):

- the outer surface of the heart;
- left atrium;
- left ventricle;
- right atrium;
- right ventricle;
- mitral valve;
- tricuspid valve;
- atrioventricular node;
- sinoatrial node;
- His bundle;
- Bachmann bundle;
- Signal ways.

We use the heart surface polygonal model to generate a tetrahedral FE model. We can vary the total number of vertices and tetrahedrons in the FE model.

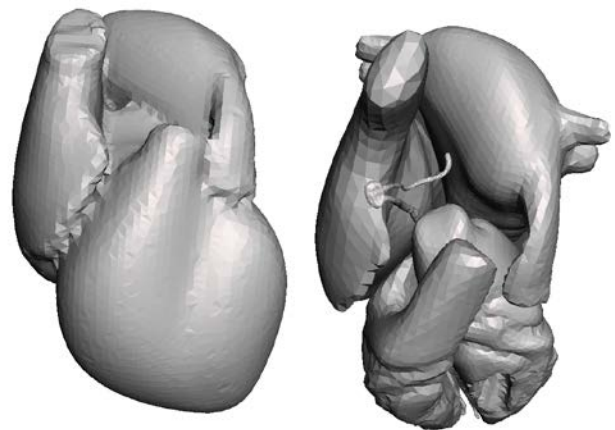


Fig. 1 The outer surface of the heart and inner tissues.

3. Algorithm of model generation

The algorithm consists of several parts: FE model generation; classification of atriums and ventricles; removal of cavities; cardiovascular system classification.

Step 1. Generation of the FE model.

Generation of a three-dimensional finite element mesh is labour-intensive process, that is why there are few high-quality open-source 3D mesh generators. We used Netgen for mesh generation, because Netgen is an open-source framework with LGPL v2 license, it is well-tested, and has its own user community. Netgen uses the outer surface of the heart in stl format, and yields a FE model consisting of tetrahedrons (Figure 2).

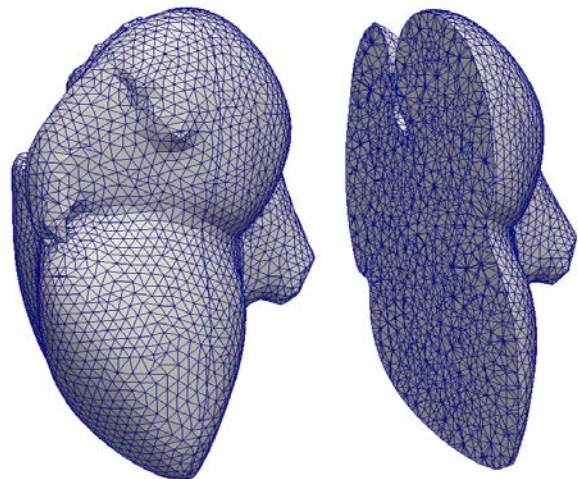


Fig. 2 Generated FE-model

Step 2. Removing tetrahedrons of atria and ventricles cavities.

After the first step we have the FE model, which consists of tetrahedrons inside atria and ventricles cavities and we delete them. To remove them we need to mark vertices for deleting. We mark vertices located inside tissue meshes (Figure 1) via the ray casting algorithm (J. D. Foley, 1990). A two-dimensional version of the algorithm is shown in Figure 3.

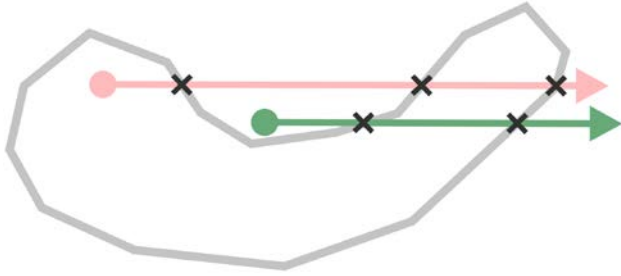


Fig 3 Even-rule algorithm (2D schema). If the point is on the inside of the polygon then it will intersect the edge an odd number of times, and outside otherwise.

We start the ray from a tested vertex in any fixed direction and calculate the number of intersections with heart tissue shells. If the point is outside of the shell the ray will intersect it an even number of times. If the point is inside the shape then the ray will intersect the edge an odd number of times.

Having tested vertices with all shapes, we can delete tetrahedrons consisting of marked vertices. After deleting we obtain the model shown in Figure 4.

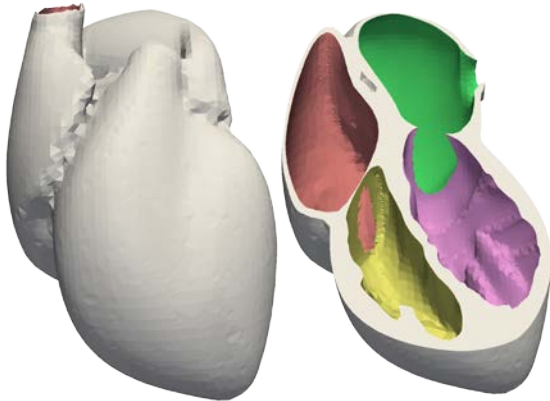


Fig. 4 FE-model with removed cavities

Step 3. Marking up the electrical conduction system of the heart.

To mark up the cardiac conduction system we use the ray casting algorithm for checking whether the point is inside or outside the shell again. As a result we have a model with marked atriums, ventricles and cardiac conduction system.

4. Parallel realization

The brunt of the calculation is marking points according to tissue type. We calculate it with the ray casting algorithm. This algorithm is good for parallel calculations, because we can test a lot of points with the same shell together. Parallel realization of the ray casting algorithm: we divide all vertices into blocks whose size equals size of the GPU thread block and perform calculations for blocks independently; inside the block, the ray casting algorithm is performed for all vertices simultaneously.

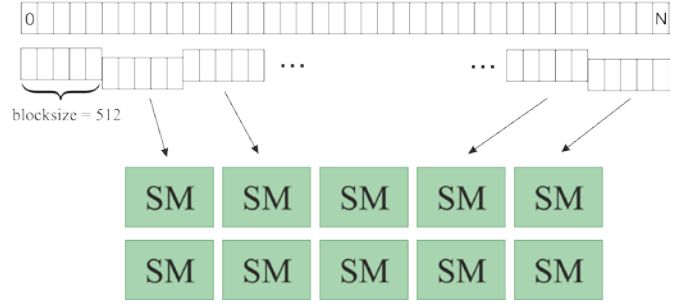


Fig. 5 Data parallelization scheme for the ray casting algorithm. SM - Streaming Microprocessor

Parallelization scheme is shown in Figure 5. All vertices are divided into blocks of the same size. On a GeForce GTX 680 (GK104), the optimal block size was found to be 512 threads. Scheduler allocates vertex blocks for processing on Streaming Multiprocessors automatically.

As the maximum length of the tetrahedron edge decreases, the number of vertices and tetrahedrons and the time for their processing increase exponentially (Figure 6), and it takes more than 6 hours for sequential algorithm to process 2 million vertices.

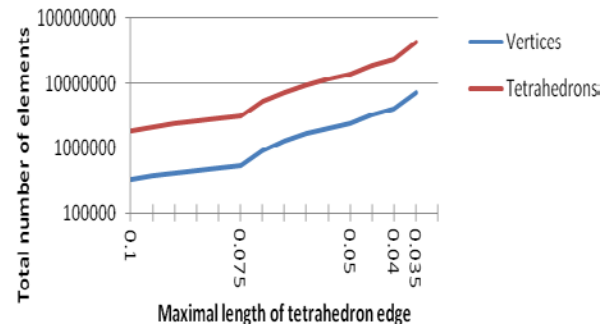


Fig. 6 Ratio between the length of tetrahedron edge and the number of elements. Y axis has logarithmic scale

We used CUDA for the parallel version. To measure the performance, a computer with the following characteristics was used: CPU Intel Core-i7 3820 3.6 GHz and GPU Nvidia GTX 680 4Gb 1006 MHz 1536 cores. The results are shown in the table below. Algorithms were tested on a mesh consisted of 2389529 vertices and 13690149 tetrahedrons.

Table 1: Speed-up of the ray casting algorithm with CUDA

Type of shape	Count of triangles	CPU msec	CUDA msec	Speed-up
AV	328	30995	100	310
SAV	590	54228	165	328
SA	792	82990	223	372
B	830	74979	221	339
F	2454	222461	606	367
RA	2646	247647	645	383
RV	3026	329501	771	427
His	4216	449535	1044	430
LA	5686	473853	1318	359
LV	7180	714429	1735	411
Total	27748	26800618	6828	392

We can see from the table that the speed-up when using the CUDA realization of the algorithm compared to the serial version is about 400x. Accelerating structures will increase the speed of the algorithm even more.

5. Conclusions

Having completed all the steps of the algorithm, we obtain a model of the heart, consisting of elements that belong to one of 10 types of tissue, to simulate the propagation of electrical heart signals along conductive paths of the cardiac system. With an optimized algorithm we can easily update our mesh after each tissue model correction, because the updating process takes some minutes rather than hours as is the case with sequential algorithms.

6. Acknowledgements

The Authors acknowledge Ministry of Education and Science of Russia (Contract № 02.G25.31.0157).

References

- Arevalo HJ, B. P. (2016). Computational rabbit models to investigate the initiation, perpetuation, and termination of ventricular arrhythmia. *Progress in biophysics and molecular biology* , 185–194.
- Aslanidi OV, N. T. (2013). Application of micro-computed tomography with iodine staining to cardiac imaging, segmentation, and computational model development. . *IEEE Trans Med Imaging.* , 32-8.
- Colli Franzone P, G. L. (1998). Spread of excitation in 3-D models of the anisotropic cardiac. *Effects of fiber architecture and ventricular geometry* , 131-71.
- Deng D, J. P. (2012). An image-based model of the whole human heart with detailed anatomical structure and fiber orientation. . *Comput Math Methods Med.* , 2012-16.
- J. D. Foley, A. v. (1990). *Computer Graphics: Principles and Practice. The Systems Programming Series.* Addison-Wesley, Reading.
- Lopez-Perez, A., & Sebastian, R. (2015). Three-dimensional cardiac computational modelling: methods, features and application. *BioMedical Engineering OnLine* .
- P. Lamata et al. (2014). An automatic service for the personalization of ventricular cardiac meshes. *J. R. Soc. Interface* .
- Plastic boy store. (n.d.). Retrieved august 2017, from Plastic boy anatomy models store: <http://www.plasticboy.co.uk/store/>
- Plotkowiak M, R. B. (2008). High performance computer simulations of cardiac electrical function based on high resolution MRI datasets. *Int Conf Comput Sci 2008* , 571-80.
- R. Bordasa, K. G. (2011). Rabbit-Specific Ventricular Model of Cardiac Electrophysiological Function including Specialized Conduction System. *Prog Biophys Mol Biol* .
- Sermesant M, M. P.-M. (2006). Cardiac function estimation from MRI using a heart model and data assimilation: advances and difficulties. *Med Image Anal* , 642–56.