

INTERNATIONAL SCIENTIFIC JOURNAL

MATHEMATICAL MODELING

YEAR VIII, - ISSUE 3/2024
ISSN (PRINT) 2535-0986
ISSN (WEB) 2603-2929

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

INTERNATIONAL EDITORIAL BOARD

EDITOR I CHIEF

Assoc. Prof. D.Sc. Milena Racheva
Technical University of Gabrovo

BG

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
Galia Angelova, Prof. DSc,	Bulgarian Academy of Science	BG
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. Mendeleyev Institute for Metrology (VNIIM)	RU
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
Renat Sadykov, Prof.	Kazan State Power Engineering University	RU
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 VIII, ISSUE 3 / 2024

All articles are published after peer review by two independent reviewers.

EDITOR IN CHIEF:

Assoc. Prof. D.Sc. Milena Racheva
Technical University of Gabrovo

CONTENTS

THEORETICAL FOUNDATIONS AND SPECIFICITY OF MATHEMATICAL MODELLING

Optimization approach to neutron spectra unfolding with Bonner multi-sphere spectrometer Alexei Chizhov, Konstantin Chizhov	89
On the Fourier Transform for Periodic Functions Milena Racheva	91

MATHEMATICAL MODELLING OF TECHNOLOGICAL PROCESSES AND SYSTEMS

Analysis and comparison of steam turbines from older and newer power plant Mrzljak Vedran, Poljak Igor, Prpić-Oršić Jasna, Lorencin Ivan	94
Determination Of Physico-Chemical Parameters Of Hydrocarbon Gas Based On Field Data. Lusjen Ismaili	98
Modeling of Shredding Blade for Nonwoven Waste Fabric Enes Bitigen, Ali H. Nazik, Tahsin Topbaşoğlu, Onur Çimen, İ.Etem Saklakoğlu	101
Mathematical modeling of aluminum alloys Adelina Miteva, Margarita Dimitrova	104
Solution of the system of equations of energy and mass transfer with account of volumetric heat sources Renat A. Sadykov, Airat L. Osipov, Artem V. Akhmerov	108

MATHEMATICAL MODELLING OF SOCIO-ECONOMIC PROCESSES AND SYSTEMS

Educational Support by Grandparents and Human Capital Growth: An OLG Model with Endogenous Time Allocation Mauro Maria Baldi, Raffaella Coppier, Elisabetta Michetti	110
Applicability of cable theory to study of action potential propagation in cardiac tissue Natela Zirakashvili	114

MATHEMATICAL MODELLING OF MEDICAL-BIOLOGICAL PROCESSES AND SYSTEMS

Bayesian vs. frequentist inference – an ophthalmic study on ocular perfusion pressure Biljana Tojtovska, Panche Ribarski, Antonela Ljubic, Galina Dimitrova	118
---	-----

Optimization approach to neutron spectra unfolding with Bonner multi-sphere spectrometer

Alexei Chizhov¹, Konstantin Chizhov^{2,3}

Laboratory of Radiation Biology, Joint Institute for Nuclear Research, Dubna, Russian Federation¹

Meshcheryakov Laboratory of Information Technology, Joint Institute for Nuclear Research, Dubna, Russian Federation²

Dubna State University, Dubna, Russian Federation³

chizhov@jinr.ru; kchizhov@jinr.ru

Abstract: For unfolding neutron spectra at physical accelerator facilities in a very wide energy range, Bonner multi-sphere spectrometers are effectively used. Such spectrometers consist of a thermal neutron detector placed in spherical polyethylene moderators of various diameters which are characterized by certain sensitivity functions. The report proposes an approach to optimizing the choice of the number and size of spheres for conducting rational measurements and subsequent unfolding of neutron spectra using Tikhonov's regularization method. Our approach is based on the use of weighting factors in the regularization functional, built on the condition numbers of the Gram matrix of the set of sensitivity functions. The effectiveness of the approach is demonstrated using the spectral unfolding of reference neutron fields of the JINR Phasotron.

Keywords: NEUTRON SPECTRUM, BONNER SPECTROMETER, SENSITIVITY FUNCTION, FREDHOLM EQUATION, TIKHONOV REGULARIZATION METHOD

1. Introduction

At high-energy accelerators, measurement of neutron spectra with a Bonner multi-sphere detector [1] for radiation monitoring purposes is a basic technique. The spectrometer consists of a set of spherical polyethylene moderators of different diameters and a thermal neutron sensor inside them. The method is based on the dependence of the neutron moderation length on their energy, i.e. the dependence of the spectrometer sensitivity on the size of the moderators. The use of different combinations of moderator spheres and thermal sensors allows a wide range of energies to be covered, with each set peaking at a specific neutron energy. The energy dependences of the sensitivity (response) functions for moderators of different diameters have different extended shapes with mutual intersections, e.g., as in Fig. 1. In this report, we propose a numerical approach to unfolding neutron spectra based on their expansion in terms of detector sensitivity functions, using A.N. Tikhonov's regularization [2], in which the stabilizing functional is selected with a specific weight matrix to provide statistical balancing of contributions from measurements with spheres of different diameters. Using the example of spectral unfolding of the JINR Phasotron reference neutron fields, we show that the concept of a weight matrix makes it possible to select optimal sets of moderator spheres for performing effective measurements of neutron spectra.

2. Neutron Fluence Spectrum Unfolding Using Bonner Spectrometers Based on Sensitivity Function Decomposition

Neutron fluence spectrum $\varphi(E)$ can be obtained from Bonner spectrometer measurements using an unfolding algorithm that solves a problem described by the system of M Fredholm's integral equations of the first kind:

$$\begin{cases} \int_{E_{\min}}^{E_{\max}} K_1(E)\varphi(E)dE = Q_1, \\ \vdots \\ \int_{E_{\min}}^{E_{\max}} K_M(E)\varphi(E)dE = Q_M, \end{cases} \quad (1)$$

where Q_j is the count rate reading of the Bonner thermal detector with the j -th sphere; $K_j(E)$ is the kernel of the j -th equation, which is a function of the sensitivity (response) of the detector to neutrons of various energies; M is the number of spheres used to measure the spectrum [3]. The integration limits $E_{\min}$ and $E_{\max}$ are determined by the spectrum definition area and the set of detectors used for measurements. In our analysis, we used the sensitivity functions from [4] corresponding to the spectrometer without a moderator sphere and 7 options with moderator spheres of diameters 2, 3, 5, 8, 10, 12, 18 inches, which are shown in Fig. 1.

Since the energy range exceeds several orders of magnitude, it is therefore convenient to use a new dimensionless energy variable called lethargy $u(E) = \lg(E/E_{\min})$. Then in terms of the new variable $u(E)$ the integral equations (1) take the form

$$\ln 10 \times \int_0^{\lg(E_{\max}/E_{\min})} K_j(u) \cdot \varphi(u) E(u) du = Q_j, \quad j = 1, \dots, M. \quad (2)$$

Therefore, instead of the spectrum $\varphi(E)$, it is more rational to find its product $\varphi(u)E(u)$.

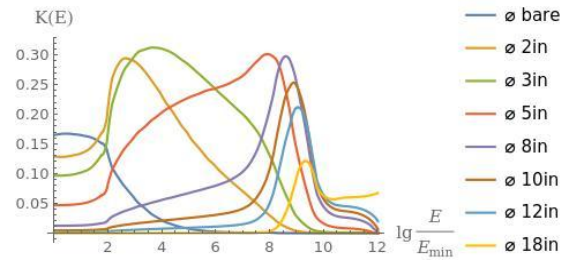


Fig. 1. Sensitivity (response) functions for Bonner spectrometer without sphere (bare), and with spheres of diameters 2, 3, 5, 8, 10, 12, 18 inches ($E_{\min} = 4.64 \cdot 10^{-9}$ MeV) [4].

Our approach to finding the product $\varphi(u)E(u)$ is to expand it into sensitivity functions $K_j(u)$ of the Bonner spectrometers used for measurements

$$\Phi(u) \equiv \varphi(u)E(u) = \sum_{j=1}^M C_j \cdot K_j(u), \quad (3)$$

and thereby determine the unknown expansion coefficients C_j using the system of equations (2). As a result, to find C_j we obtain a system of M linear algebraic equations, represented in the matrix form as

$$\mathbf{AC} = \mathbf{Q}, \quad (4)$$

where elements of symmetric matrix $\mathbf{A}_{M \times M}$ read as

$$A_{ij} = \ln 10 \times \int_0^{\lg(E_{\max}/E_{\min})} K_i(u) \cdot K_j(u) du, \quad (5)$$

and M -dimensional vectors $\mathbf{C}^T = (C_1, \dots, C_M)$ and $\mathbf{Q}^T = (Q_1, \dots, Q_M)$. The matrix $\mathbf{A}$ is ill-conditioned, and therefore direct solving such a system of equations by inverting the matrix $\mathbf{A}$ does not provide a physically justified solution for the spectrum.

3. Tikhonov Regularization Method with Weight Coefficients

We construct solution (4) based on Tikhonov's regularization method, which is generalized taking into account the significance of the contributions of different detectors to the measurement process. As such a criterion, we used the condition numbers of the matrices

A_j ($j = 1, \dots, M$), obtained from the Gram matrix $A_{M \times M}$ (5) of the set of sensitivity functions by deleting the j -th row and j -th column, from which the elements of the diagonal matrix $W = \{W_{jj}\}$ are constructed:

$$W_{jj} = \text{cond}(A_j) = \lambda_{\max}(A_j) / \lambda_{\min}(A_j), \quad (6)$$

where $\lambda(A_j)$ are the eigenvalues of the matrix A_j . The matrix W plays the role of a weight matrix in constructing the stabilizing functional in Tikhonov's regularization algorithm

$$\begin{aligned} M_W^\alpha[C] &= (AC - Q)^T W (AC - Q) \\ &\quad + \alpha \int_0^{\lg(\frac{E_{\max}}{E_{\min}})} \{\Phi^2(u) + [\Phi'(u)]^2\} du \\ &= \sum_{j=1}^M W_{jj} (\sum_{i=1}^M A_{ji} C_i - Q_j)^2 + \alpha \sum_{i,k=1}^M C_i C_k \int_0^{\lg(\frac{E_{\max}}{E_{\min}})} \{K_i(u) \cdot \\ &\quad K_k(u) + K_i'(u) \cdot K_k'(u)\} du, \end{aligned} \quad (7)$$

where α is the regularization parameter. From the condition for the minimum of this functional

$$\partial M_W^\alpha[C] / \partial C_i = 0 \quad (8)$$

we arrive at a linear algebraic system of equations of the matrix form

$$[AWA + \alpha(A + B)]C^\alpha = AWQ, \quad (9)$$

where elements of symmetric matrix $B_{M \times M}$ have the form

$$B_{ij} = \ln 10 \times \int_0^{\lg(\frac{E_{\max}}{E_{\min}})} K_i'(u) \cdot K_j'(u) du. \quad (10)$$

The choice of the regularization parameter α is carried out in accordance with the generalized residual principle, i.e. is found from the equation

$$(AC^\alpha - Q)^T (AC^\alpha - Q) - \delta^2 Q^T Q - \mu^2(Q, A) = 0, \quad (11)$$

where δ is the relative error in measurements of the neutron spectrum $\varphi(E)$, and $\mu(Q, A)$ is a measure of the incompatibility of the system of equations (1) taking into account physical restrictions on the spectrum form. As a result of such fixation of the parameter α , the neutron spectrum (3) is represented in the form

$$\Phi^\alpha(u) \equiv \varphi^\alpha(u)E(u) = \sum_{j=1}^M C_j^\alpha \cdot K_j(u). \quad (12)$$

Having obtained the neutron spectrum (12), it is possible to estimate the radiation dose rate $\dot{H}^\alpha$ corresponding to this neutron field using the formula

$$\dot{H}^\alpha = \int_{E_{\min}}^{E_{\max}} h(E) \cdot \varphi^\alpha(E) dE = \ln 10 \times \int_0^{\lg(\frac{E_{\max}}{E_{\min}})} h(u) \cdot \Phi^\alpha(u) du, \quad (13)$$

where $h(E)$ are the dose conversion coefficients for external radiation.

4. Unfolding Neutron Spectra at the JINR Phasotron by Different Sets of Moderator Spheres

In accordance with the proposed method for finding weighting factors (6), for sensitivity functions from [4] we obtain the following values (normalized to the largest one)

$$W = \{1.00, 0.69, 0.43, 0.28, 0.07, 0.02, 0.03, 0.18\}. \quad (14)$$

From the given values of this weight matrix (14) it follows that detector 1 makes the main contribution to the measurements, while the contribution of detectors 5, 6 and 7 is rather insignificant.

To demonstrate the effectiveness of the Bonner spectrometer sphere set selection based on the weight matrix, we considered four variants of neutron spectra reconstruction, namely: for the full sphere set using the standard Tikhonov regularization method [5]

and with the weight matrix, as well as excluding the bare sensor and the set of 5, 6, 7 spheres.

The results of unfolding of the neutron spectra for two locations of the JINR Phasotron [6]: the reference neutron field in the labyrinth of the tunnel in the basement under the main hall of the accelerator ("soft" field) and the reference field behind the two-meter concrete shield of the Phasotron ("hard" field) are shown in Fig. 2.

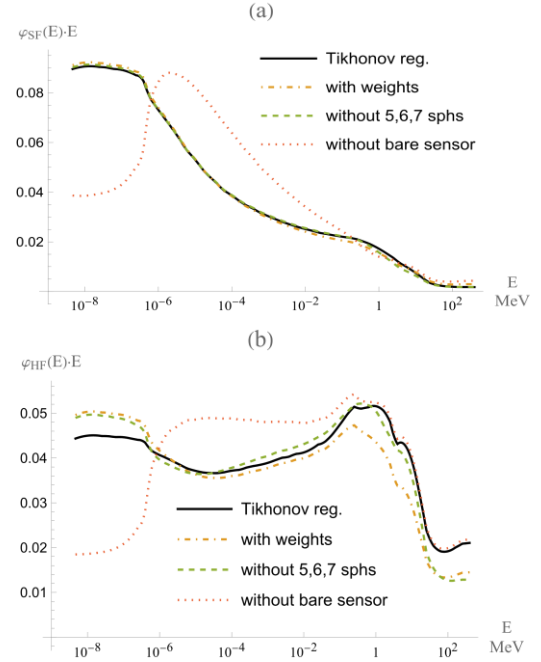


Fig. 2. Reconstructed neutron spectra for the "soft" (a) and "hard" (b) radiation fields of the JINR Phasotron with the relative measurement error $\delta = 0.05$ (5%).

The figure shows that for the measured spectra there is good agreement between the results obtained both by the standard regularization method and with the weight matrix with the full set of spheres, and with the exclusion of spheres 5, 6, 7 with the smallest contribution. Whereas the exclusion of the significant detector 1 greatly changes the reconstruction result. Thus, the weight matrix constructed by the method (6) can be used to determine the optimal set of spheres.

5. Conclusion

In the report we proposed the approach to unfolding neutron spectra with a weight matrix in the regularization algorithm of A.N. Tikhonov. It is constructed on the basis of taking into account the mutual behavior of the sensitivity functions of the Bonner multi-sphere spectrometer depending on energy. Such an approach provides statistical balancing of contributions from measurements with moderator spheres of different diameters, which allows theoretically determining optimal sets of Bonner spheres (their sizes and number) for effective practical measurements.

6. References

1. R.L. Bramblett, R.I. Ewing, T.W. Bonner, *Nuclear Instruments and Methods*, **9**, 1-12 (1960)
2. A.N. Tikhonov, *Reports of the USSR Academy of Sciences*, **153**, 49-52 (1963) (in Russian)
3. K. Chizhov, L. Beskrovnaya, A. Chizhov, *Physics of Particles and Nuclei*, **55**, 532-534 (2024)
4. M. Awschalom, R.S. Sanna, *Radiation Protection Dosimetry*, **10**, 89-101 (1985)
5. A. Chizhov, K. Chizhov, *Mathematical Modeling*, **7**, 62-64 (2023)
6. V. Aleinikov, V. Bamblevskij, M. Komochkov, A. Krylov, Y. Mokrov, G. Timoshenko G, *Radiation Protection Dosimetry*, **54**, 57-59 (1994)

On the Fourier Transform for Periodic Functions

Milena Racheva
 Technical University of Gabrovo, Bulgaria
 milena@tugab.bg

Abstract: The paper deals with some aspects of the presentation and application of periodic time-dependent functions in the Fourier analysis. Different approaches for defining and utilising periodic functions are considered. The case when one has only a discrete set of values obtained from measurement and the function itself is not known is also included. In general, the type and the shape of the corresponding frequency distribution is a point of interest and discussion. The paper presents numerous examples which illustrate the proposed ideas.

Keywords: PERIODIC FUNCTION, FOURIER DENSITY/DISTRIBUTION, DIRAC FUNCTION, APPROXIMATION

1. Introduction

When we talk about the relationship between the time function $x(t)$ and its frequency distribution $X(f)$ by means of Fourier transformation [1]:

$$X(f) = \int_{-\infty}^{+\infty} x(t) e^{-2\pi f i t} dt, \quad (1)$$

it is usually means that the signal $x(t)$ is a non-periodic function or a function with a very large period. Such a problem arises in physics and for some engineering sciences.

There are some apparent restrictions. For example, convergence of $\int_{-\infty}^{+\infty} x(t) dt$ or requirement that the function concerned to approach zero as the variable t approaches $\pm\infty$. These restrictions obviously are not fulfilled by the periodic functions. We will see that a sophisticated theory of generalized functions can help us here.

We could consider the Fourier transform of a T -periodic function in local sense, i.e. when the function is in any interval with range T . If a signal is of duration τ and the period T is much larger than τ ($T \gg \tau$), then we are interested in the local Fourier transform.

Relationships between original function $x(t)$ and its Fourier image $X(f)$ can be noted by [1,2]:

$$x(t) \leftrightarrow X(f) = F(x(t)). \quad (2)$$

Our research focuses on two questions: how to define a periodic function and how to obtain its Fourier transform.

2. Introducing a Periodic Function

Let us consider the T -periodic function $x(t)$. A key role in its definition and further use is played by the Dirac delta function δ . This generalized function induces another function of such type called “shah function” [2,3] (Fig. 1):

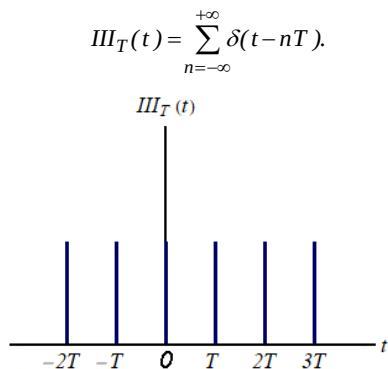


Fig. 1 Function $III_T(t)$

It is also known as “Dirac comb”.

The corresponding Fourier transform is another Dirac comb function [3,4]:

$$F(III_T(t)) = \sum_{n=-\infty}^{+\infty} X_n \delta(f - n f_0),$$

where f_0 is the essential frequency, $f_0 = \frac{1}{T}$, and $X_n = f_0$.

Then from notation (2) we have (Fig. 2):

$$III_T(t) \leftrightarrow f_0 III_{f_0}(f).$$

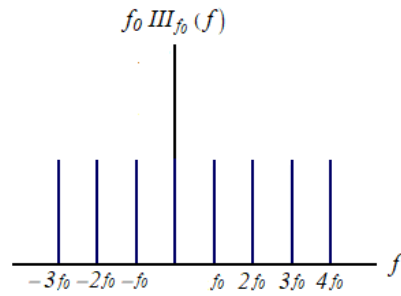


Fig. 2 The image of $III_T(t)$

In order to introduce the periodic function $x(t)$, we consider the function $\tilde{x}(t)$:

$$\tilde{x}(t) = \begin{cases} x(t), & -\frac{T}{2} \leq t \leq \frac{T}{2}, \\ 0, & \text{elsewhere.} \end{cases}$$

Then we use the convolution theorem [5]:

$$x(t) = III_T(t) * \tilde{x}(t).$$

Indeed:

$$\begin{aligned} III_T(t) * \tilde{x}(t) &= \int_{-\infty}^{+\infty} \tilde{x}(t) III_T(t-u) du \\ &= \sum_{u=-\infty}^{+\infty} \int_{-\infty}^{+\infty} \tilde{x}(t) \delta(t-u-nT) du = \sum_{n=-\infty}^{+\infty} \tilde{x}(t-nT) \end{aligned}$$

So, $x(t)$ is a T -periodic copy of $\tilde{x}(t)$.

Another approach to define a periodic function is for instance is considered in Example 1.

Example 1: Consider the following function (Fig. 3):

$$x(t) = \begin{cases} 2-2t, & 0 \leq t \leq 1, \\ t-1, & 1 \leq t \leq 2, \\ \text{periodic elsewhere.} \end{cases}$$

Here we give Wolfram Language Code:

```
T=2;
x[t_./;0<=t<=2]:=Piecewise[{{2-2 t,0<= t<=1},{t-1,1<=t<=2}}]
x[t_]:=x[Mod[t,T]]
```

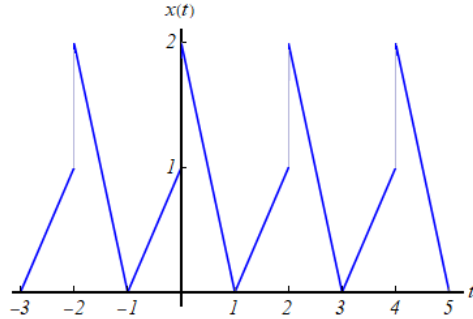


Fig. 3 The function from Example 1

3. Fourier Transform of Periodic Function

We cannot use definition (1) for the T -periodic function $x(t)$ because the integral is not convergent. Therefore, we will use approximation of a periodic function by the corresponding Fourier series.

From sine and cosine Fourier images [1,2]:

$$\cos(2\pi f_0 t) = \frac{1}{2}(e^{i2\pi f_0 t} + e^{-i2\pi f_0 t}) \leftrightarrow \frac{1}{2}[\delta(f - f_0) + \delta(f + f_0)],$$

$$\sin(2\pi f_0 t) = \frac{1}{2i}(e^{i2\pi f_0 t} - e^{-i2\pi f_0 t}) \leftrightarrow \frac{1}{2i}[\delta(f - f_0) - \delta(f + f_0)],$$

we get

$$x(t) = \sum_{n=-\infty}^{+\infty} X_n \delta(f - nf_0), \quad (3)$$

where $f_0 = \frac{1}{T}$ and X_n are complex Fourier coefficients

$$X_n = f_0 \int_T x(t) e^{-i2\pi f_0 n t} dt. \quad (4)$$

The graph of the frequency distribution function is monotonically decreasing in size bars ($|X_n| \rightarrow 0$ as $n \rightarrow \pm \infty$).

Example 2: Let us use the 2-periodic function from Example 1.

Here $f_0 = \frac{1}{2}$ and from (3) and (4) we obtain:

$$\begin{aligned} X_n &= \frac{1}{2} \int_{-1}^0 (t+1) e^{-i\pi n t} dt + \frac{1}{2} \int_0^1 (2-2t) e^{-i\pi n t} dt \\ &= -\frac{3+2e^{-i\pi n} + e^{i\pi n} + i\pi n}{2n^2 \pi^2}, \quad n=1,2,\dots \end{aligned}$$

Now, we will develop the idea proposed by the author in [6]. Often in engineering practice we have data obtained after

measurement and the periodic function $x(t)$ is unknown. The next two examples illustrate the proposed approach, which is based on approximation of the function $x(t)$.

Example 3: For the function $x(t)$ the following data are known given in Table 1.

j	t_j	$x(t_j)$
0	-0.98	0.04
1	-0.63	0.21
2	-0.44	0.48
3	-0.19	0.78
4	-0.05	0.95
5	0.1	1.99
6	0.23	1.54
7	0.45	1.08
8	0.73	0.32
9	0.97	0.1

Table 1: The values of $x(t)$

X_1	$0.365677 - 0.170446 i$
X_2	$0.032305 - 0.096418 i$
X_3	$0.02932 - 0.055125 i$
X_4	$0.038056 - 0.056636 i$
X_5	$0.010229 - 0.046577 i$
X_6	$0.019381 - 0.038798 i$
X_7	$0.005173 - 0.036179 i$
X_8	$0.011388 - 0.029371 i$
X_9	$0.003118 - 0.029095 i$

Table 2: The Fourier coefficients approximately obtained using Lagrange interpolation of $x(t)$

We approximate the function $x(t)$ by Lagrange interpolation, dividing into two parts – on the intervals $[t_0, t_4]$ and $[t_5, t_9]$. Thus, on these two intervals the function $x(t)$ is interpolated by fourth-order polynomials $L_{4,1}(t)$ and $L_{4,2}(t)$, respectively.

Let us denote $L_4(t) = \begin{cases} L_{4,1}(t), & -1 \leq t \leq 0, \\ L_{4,2}(t), & 0 < t \leq 1, \end{cases}$ (see Fig. 4).

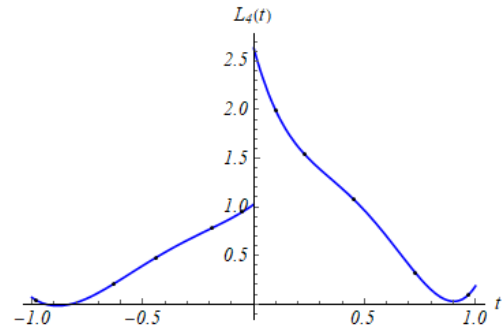


Fig. 4 The approximation function $L_4(t)$

Substituting in (4) $x(t)$ by its interpolant $L_4(t)$ (here $T = 2$), one may easily calculate the Fourier coefficients X_n , $n=1,2,\dots$ (see Table 2).

Example 4: For the function $x(t)$ from Example 3 we undertake approximation by least squares method. Two variants are implemented – approximation of the data given in Table 1 by linear as well as quadratic functions. Again, the approximations, which are shown in Fig. 5, are separately obtained in intervals $[t_0, t_4]$ and $[t_5, t_9]$.

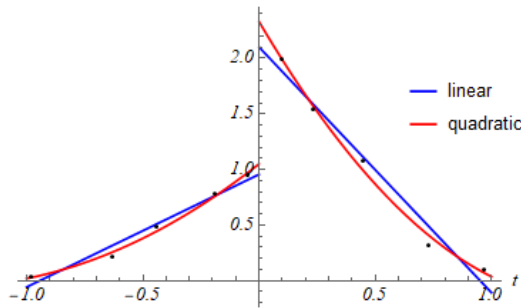


Fig. 5 The approximations of $x(t)$ by least squares method

Thus, substituting in (4) $x(t)$ by approximate linear/quadratic function obtained using least squared method, it is easy to get the corresponding Fourier coefficients X_n , $n=1,2,\dots$ (Table 3 and Table 4).

X_1	$0.32665 - 0.174355 i$
X_2	$0. - 0.095158 i$
X_3	$0.036294 - 0.058118 i$
X_4	$0. - 0.047579 i$
X_5	$0.013066 - 0.034871 i$
X_6	$0. - 0.031719 i$
X_7	$0.006666 - 0.024908 i$
X_8	$0. - 0.02379 i$
X_9	$0.004033 - 0.019373 i$

Table 3: The Fourier coefficients obtained using linear approximation of $x(t)$

X_1	$0.336937 - 0.164888 i$
X_2	$0.047551 - 0.100563 i$
X_3	$0.037437 - 0.067267 i$
X_4	$0.011888 - 0.050281 i$
X_5	$0.013477 - 0.040951 i$
X_6	$0.005283 - 0.033521 i$
X_7	$0.006876 - 0.029367 i$
X_8	$0.002972 - 0.025141 i$
X_9	$0.00416 - 0.022878 i$

Table 4: The Fourier coefficients obtained using quadratic approximation of $x(t)$

4. Conclusion

Important aspects in signal processing and frequency distribution of periodic function are presented. The crucial role in these applications falls to the generalized Dirac delta function. In this work, it is shown that approximate methods in engineering research are also possible.

Acknowledgements. This work is partially supported by the University Project **2404S** "Applied mathematical research on energy and economic efficiency of electrical equipment in the conditions of energy transition", financed by the Ministry of Education and Science of the Republic of Bulgaria and by the European Regional Development Fund under the Operational Program "Scientific Research, Innovation and Digitization for Smart Transformation 2021-2027", Project CoC "Smart Mechatronics, Eco- and Energy Saving Systems and Technologies", **BG16RFPR002-1.014-0005**.

5. References

1. M. Racheva, *Applied Mathematics*, Vasil Aprilov – Gabrovo (2018)
2. D. Jordan, P. Smith, *Mathematical techniques: An introduction for the engineering, physical, and mathematical sciences*. OUP Oxford (2008)
3. M.J. Lighthill, *An introduction to Fourier analysis and generalised functions*. Cambridge University Press (1958)
4. A. Còrdoba, A. Dirac combs. Letters in mathematical physics, 17: 191-196 (1989)
5. R. Bracewell, P.B. Kahn, The Fourier transform and its applications. American Journal of Physics, 34(8), 712-712 (1966)
6. Racheva M. Discrete data approximations and their application in engineering research, International Scientific Conference UNITECH 2023, 17-18 November 2023, Gabrovo, Bulgaria, II 246 – II 249

Analysis and comparison of steam turbines from older and newer power plant

Mrzljak Vedran¹, Poljak Igor², Prpić-Oršić Jasna¹, Lorencin Ivan³

¹Faculty of Engineering, University of Rijeka, Vukovarska 58, 51000 Rijeka, Croatia

²Department of maritime sciences, University of Zadar, Mihovila Pavlinovića 1, 23000 Zadar, Croatia

³Faculty of Informatics, Juraj Dobrila University of Pula, Rovinjska 14, 52100 Pula, Croatia

E-mail: vedran.mrzljak@riteh.uniri.hr, ipoljak1@unizd.hr, jasna.prpic.orsic@riteh.uniri.hr, ivan.lorencin@unipu.hr

Abstract: In the presented paper are performed energy and exergy analyses as well as a comparison of two similar steam turbines from conventional power plants. The first turbine is from an older, while the second turbine is from newer steam power plant. The dominant mechanical power producer in an older steam turbine is LPC (which produces mechanical power of almost 66 MW), while in a newer steam turbine the dominant mechanical power producer is IPC which produces power equal to 102.4 MW. Whole older steam turbine has higher energy and exergy loss in comparison to the whole newer steam turbine. Whole turbine from the newer power plant has much higher energy and exergy efficiencies in comparison to whole turbine from an older power plant. In an older steam turbine, LPC did not show the expected performance because its exergy efficiency is very low (equal to 75.49%), what is much lower than in any other cylinder from both observed turbines. The ambient temperature change sensitivity of the two observed steam turbines and their cylinders is reverse proportional to efficiencies (both energy and exergy). Steam turbine from an older power plant is much more sensitive to the ambient temperature change.

KEYWORDS: STEAM TURBINE, ENERGY AND EXERGY ANALYSES, PERFORMANCE COMPARISON, OLDER AND NEWER POWER PLANT, THE AMBIENT TEMPERATURE SENSITIVITY

1. Introduction

The majority of electrical energy nowadays is produced by the steam turbines [1]. There are a variety of power plants in which steam turbines are used, such as conventional steam power plants, nuclear power plants, as well as supercritical and ultra-supercritical steam power plants [2-4]. Steam turbines also have an important role as a part of combined-cycle power plants and in cogeneration power plants for simultaneous production of electrical energy and heat [5]. Along with the mentioned, steam turbines can also be found in the marine steam propulsion plant as the main mechanical power producers for ship propulsion [6], as well as auxiliary turbines [7].

Steam turbines are usually complex components composed of several cylinders [8]. Only auxiliary steam turbines (such as turbo-generators or steam turbines for the drive of pumps or compressors) dominantly have only one cylinder because auxiliary steam turbines are low-power turbines [9].

In this paper are performed energy and exergy analyses as well as a comparison of two similar steam turbines from conventional power plants. The first turbine is from an older, while the second turbine observed in this analysis is from newer power plant. It is interesting to observe and compare efficiencies and losses (both energy and exergy) as well as sensitivity to the ambient temperature change of both steam turbines and their cylinders.

2. Description of the analyzed steam turbines

General scheme of the analyzed steam turbines along with operating points necessary for the energy and exergy analyses is presented in Fig. 1.

Both observed steam turbines are composed of three cylinders connected to the same shaft (HPC is a High Pressure Cylinder, IPC is an Intermediate Pressure Cylinder and the LPC is a Low Pressure Cylinder). Produced mechanical power in all the cylinders of both turbines is used for the electrical generator drive.

The first steam turbine, Fig. 1 (A) operates in an older power plant, while the second steam turbine, Fig. 1 (B) operates in newer power plant. In a steam turbine from older power plant HPC has only one steam extraction, IPC two, while LPC has three steam extractions. In a steam turbine from newer power plant, HPC has two steam extractions, IPC four and LPC only one steam extraction. Each steam extraction from each cylinder of both analyzed steam turbines lead a certain amount of steam to the components of regenerative condensing/feedwater heating system. After steam expansion in a last turbine cylinder (LPC), steam is delivered to the main condenser for condensation [10], which is valid for both analyzed steam turbines.

Also, both analyzed steam turbines have reheater mounted in a steam flow steam between HPC and IPC, which increases steam temperature before its expansion in IPC.

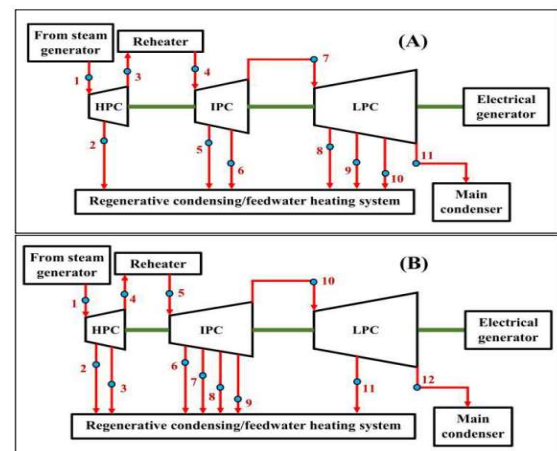


Fig. 1. General scheme of the analyzed steam turbines along with operating points required for the energy and exergy analyses and comparison; (A) = Steam turbine from older power plant; (B) = Steam turbine from newer power plant

It is essential to mention that an exergy analysis of any steam turbine (or turbine cylinder) is based on the real (polytropic) steam team expansion process which involves all the losses during expansion. Steam turbine energy analysis is based on the comparison of real (polytropic) and ideal (isentropic) expansion processes. Ideal (isentropic) steam expansion process neglects all the losses which occur during expansion, so the ideal expansion is the best one which can theoretically occur in any turbine or turbine cylinder.

Comparison of ideal (isentropic) and real (polytropic) steam expansion processes in HPC of both observed turbines is presented in Fig. 2. In a same manner are defined ideal and real steam expansion processes in all other cylinders of both observed turbines, Fig. 1.

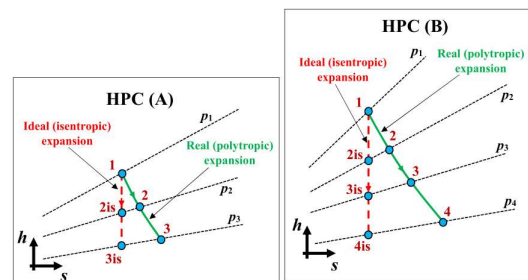


Fig. 2. Ideal (isentropic) and real (polytropic) steam expansion processes inside the HPC in h-s diagram; (A) = HPC of steam turbine from older power plant; (B) = HPC of steam turbine from newer power plant

3. Equations for the energy and exergy analyses

3.1. General equations and balances

The main energy and exergy balance equations are [11]:

$$\dot{Q}_{in} + P_{in} + \sum \dot{E}n_{in} - \dot{Q}_{out} - P_{out} - \sum \dot{E}n_{out} - \dot{E}n_L = 0, \quad (1)$$

$$\dot{X}_{in} + P_{in} + \sum \dot{E}x_{in} - \dot{X}_{out} - P_{out} - \sum \dot{E}x_{out} - \dot{E}x_L = 0, \quad (2)$$

where $\dot{Q}$ is heat energy transfer, $\dot{X}$ is a heat exergy transfer at the temperature T , P is mechanical power, index in is related to the inlet (input), index out is related to outlet (output) and index L is related to loss. $\dot{E}n$ is a total energy flow of fluid stream and $\dot{E}x$ is a total exergy flow of fluid stream which are defined by equations [12]:

$$\dot{E}n = \dot{m} \cdot h, \quad (3)$$

$$\dot{E}x = \dot{m} \cdot \varepsilon, \quad (4)$$

where $\dot{m}$ is mass flow rate, h is fluid specific enthalpy and ε is specific exergy. Specific exergy (ε) is defined by an equation [13]:

$$\varepsilon = (h - h_0) - T_0 \cdot (s - s_0), \quad (5)$$

where s is fluid specific entropy and index 0 is an index of the ambient state. Always valid mass flow rate balance for any component is [14]:

$$\sum \dot{m}_{in} = \sum \dot{m}_{out}. \quad (6)$$

3.2. Equations for the energy and exergy analyses of observed steam turbines

All the equations for the energy and exergy analyses of both steam turbines and their cylinders used in this research are developed according to guidelines and recommendations from the literature [15-17]. The equations will be presented only for the first (older) observed turbine and its cylinders, Fig. 1 (A), for a newer steam turbine and its cylinders equations are arranged in the same manner. Markings in the following equations are related to operating points from Fig. 1. In Table 1 are presented equations for the calculation of ideal (isentropic) and real (polytropic) mechanical power related to older steam turbine and its cylinders.

Table 1. Ideal (isentropic) and real (polytropic) mechanical power of an older steam turbine and its cylinders – power plant A

Component	Ideal (isentropic) mechanical power	Eq.
HPC	$P_{HPC,IS} = \dot{m}_1 \cdot (h_1 - h_{2is}) + (\dot{m}_1 - \dot{m}_2) \cdot (h_{2is} - h_{3is})$	(7)
IPC	$P_{IPC,IS} = \dot{m}_4 \cdot (h_4 - h_{5is}) + (\dot{m}_4 - \dot{m}_5) \cdot (h_{5is} - h_{6is}) + (\dot{m}_4 - \dot{m}_5 - \dot{m}_6) \cdot (h_{6is} - h_{7is})$	(8)
LPC	$P_{LPC,IS} = \dot{m}_7 \cdot (h_7 - h_{8is}) + (\dot{m}_7 - \dot{m}_8) \cdot (h_{8is} - h_{9is}) + (\dot{m}_7 - \dot{m}_8 - \dot{m}_9) \cdot (h_{9is} - h_{10is}) + (\dot{m}_7 - \dot{m}_8 - \dot{m}_9 - \dot{m}_{10}) \cdot (h_{10is} - h_{11is})$	(9)
WT	$P_{WT,IS} = P_{HPC,IS} + P_{IPC,IS} + P_{LPC,IS}$	(10)
Component	Real (polytropic) mechanical power	Eq.
HPC	$P_{HPC,PT} = \dot{m}_1 \cdot (h_1 - h_2) + (\dot{m}_1 - \dot{m}_2) \cdot (h_2 - h_3)$	(11)
IPC	$P_{IPC,PT} = \dot{m}_4 \cdot (h_4 - h_5) + (\dot{m}_4 - \dot{m}_5) \cdot (h_5 - h_6) + (\dot{m}_4 - \dot{m}_5 - \dot{m}_6) \cdot (h_6 - h_7)$	(12)
LPC	$P_{LPC,PT} = \dot{m}_7 \cdot (h_7 - h_8) + (\dot{m}_7 - \dot{m}_8) \cdot (h_8 - h_9) + (\dot{m}_7 - \dot{m}_8 - \dot{m}_9) \cdot (h_9 - h_{10}) + (\dot{m}_7 - \dot{m}_8 - \dot{m}_9 - \dot{m}_{10}) \cdot (h_{10} - h_{11})$	(13)
WT	$P_{WT,PT} = P_{HPC,PT} + P_{IPC,PT} + P_{LPC,PT}$	(14)

Equations for the calculation of energy loss and energy efficiency related to older steam turbine and its cylinders are presented in Table 2. Finally, equations for the calculation of exergy loss and exergy efficiency related to older steam turbine and its cylinders are presented in Table 3. As the exergy analysis is related to the ambient state, in this paper the base ambient state is defined with ambient pressure equal to 1 bar and ambient temperature equal to 25 °C. At the end of this analysis where is investigated the exergy efficiency sensitivity to the ambient temperature change of both observed steam turbines and their cylinders are used the same equations presented in Table 3 (the change in the ambient temperature is related to a change of specific exergies only, the equations remain the same).

Table 2. Energy loss and energy efficiency of an older steam turbine and its cylinders – power plant A

Component	Energy loss	Eq.
HPC	$\dot{E}n_{L,HPC} = P_{HPC,IS} - P_{HPC,PT}$	(15)
IPC	$\dot{E}n_{L,IPC} = P_{IPC,IS} - P_{IPC,PT}$	(16)
LPC	$\dot{E}n_{L,LPC} = P_{LPC,IS} - P_{LPC,PT}$	(17)
WT	$\dot{E}n_{L,WT} = \dot{E}n_{L,HPC} + \dot{E}n_{L,IPC} + \dot{E}n_{L,LPC}$	(18)
Component	Energy efficiency	Eq.
HPC	$\eta_{en,HPC} = \frac{P_{HPC,PT}}{P_{HPC,IS}}$	(19)
IPC	$\eta_{en,IPC} = \frac{P_{IPC,PT}}{P_{IPC,IS}}$	(20)
LPC	$\eta_{en,LPC} = \frac{P_{LPC,PT}}{P_{LPC,IS}}$	(21)
WT	$\eta_{en,WT} = \frac{P_{WT,PT}}{P_{WT,IS}}$	(22)

Table 3. Exergy loss and exergy efficiency of an older steam turbine and its cylinders – power plant A

Component	Exergy loss	Eq.
HPC	$\dot{E}x_{L,HPC} = \dot{E}x_1 - \dot{E}x_2 - \dot{E}x_3 - P_{HPC,PT}$	(23)
IPC	$\dot{E}x_{L,IPC} = \dot{E}x_4 - \dot{E}x_5 - \dot{E}x_6 - \dot{E}x_7 - P_{IPC,PT}$	(24)
LPC	$\dot{E}x_{L,LPC} = \dot{E}x_7 - \dot{E}x_8 - \dot{E}x_9 - \dot{E}x_{10} - \dot{E}x_{11} - P_{LPC,PT}$	(25)
WT	$\dot{E}x_{L,WT} = \dot{E}x_{L,HPC} + \dot{E}x_{L,IPC} + \dot{E}x_{L,LPC}$	(26)
Component	Exergy efficiency	Eq.
HPC	$\eta_{ex,HPC} = \frac{P_{HPC,PT}}{\dot{E}x_{L,HPC} + P_{HPC,PT}}$	(27)
IPC	$\eta_{ex,IPC} = \frac{P_{IPC,PT}}{\dot{E}x_{L,IPC} + P_{IPC,PT}}$	(28)
LPC	$\eta_{ex,LPC} = \frac{P_{LPC,PT}}{\dot{E}x_{L,LPC} + P_{LPC,PT}}$	(29)
WT	$\eta_{ex,WT} = \frac{P_{WT,PT}}{\dot{E}x_{L,WT} + P_{WT,PT}}$	(30)

4. Steam operating parameters required for turbines energy and exergy analyses

For each steam turbine, in each operating point presented in Fig. 1, steam operating parameters are found in [18] for an older steam turbine and in [19] for a newer steam turbine. In each operating point from the literature are known steam temperature, pressure and mass flow rate, all other steam operating parameters required in the analyses are calculated by using NIST-Refprop 9.0 software [20].

Steam operating parameters in each operating point from Fig. 1, are presented in Table 4 for an older steam turbine (power plant A) and in Table 5 for a newer steam turbine (power plant B).

Table 4. Steam operating parameters of an older steam turbine – power plant A

O.P.	Temperature (°C)	Pressure (bar)	Mass flow rate (kg/s)	Specific enthalpy (kJ/kg)	Specific entropy (kJ/kg·K)	Quality
1	535.00	133.42	133.33	3428.0	6.5446	Superheated
2	367.00	38.85	11.67	3137.7	6.6670	Superheated
3	359.00	36.64	121.67	3123.0	6.6692	Superheated
4	535.00	36.64	121.67	3529.4	7.2370	Superheated
5	418.00	16.18	2.98	3293.7	7.2912	Superheated
6	361.00	8.68	5.95	3184.1	7.4083	Superheated
7	337.21	7.24	112.74	3136.9	7.4150	Superheated
8	241.00	3.26	5.23	2948.6	7.4430	Superheated
9	155.00	1.41	6.13	2783.6	7.4743	Superheated
10	111.00	0.40	5.50	2705.2	7.8577	Superheated
11	35.50	0.06	95.88	2506.3	8.1338	0.975

O.P. = Operating point (refers to Fig. 1 (A))

Table 5. Steam operating parameters of newer steam turbine – power plant B

O.P.	Temperature (°C)	Pressure (bar)	Mass flow rate (kg/s)	Specific enthalpy (kJ/kg)	Specific entropy (kJ/kg·K)	Quality
1	540.00	131.72	176.10	3443.2	6.5687	Superheated
2	390.00	44.32	8.06	3182.7	6.6793	Superheated
3	350.20	30.03	19.37	3116.5	6.7451	Superheated
4	337.82	27.03	148.67	3094.2	6.7550	Superheated
5	541.00	25.83	148.67	3553.4	7.4249	Superheated
6	470.00	13.01	4.91	3410.7	7.5536	Superheated
7	370.20	6.63	8.31	3207.2	7.5676	Superheated
8	259.21	2.84	5.85	2987.1	7.5800	Superheated
9	177.60	1.32	6.70	2829.4	7.6100	Superheated
10	170.30	1.22	122.90	2815.5	7.6150	Superheated
11	77.00	0.41	4.59	2638.1	7.6591	Superheated
12	45.81	0.10	118.31	2488.5	7.8500	0.960

O.P. = Operating point (refers to Fig. 1 (B))

5. Results and discussion

Real mechanical power produced by both observed turbines and their cylinders is presented in Fig. 3.

When observing turbine cylinders it is clear that the dominant mechanical power producer in an older steam turbine is LPC (which produces mechanical power of almost 66 MW), while in a newer steam turbine the dominant power producer is IPC which produces mechanical power equal to 102.4 MW. It is interesting that in a newer steam turbine IPC produces more than a half of cumulative produced mechanical power in the whole turbine, regardless of the fact that IPC has four steam extractions, more than any other cylinder of both observed turbines. Observation of the whole turbines shows that older steam turbine produces cumulative mechanical power equal to 153.5 MW, while newer steam turbine produces cumulative mechanical power equal to 202.2 MW.

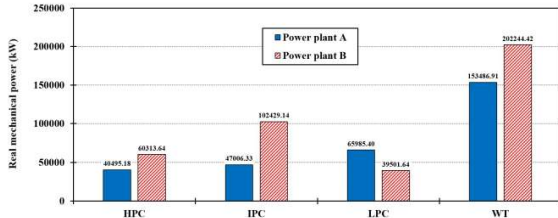


Fig. 3. Real mechanical power produced in the cylinders and in whole turbine for a steam turbine from older power plant (A) and for a steam turbine from newer power plant (B)

Energy loss of both observed turbines and their cylinders are presented in Fig. 4.

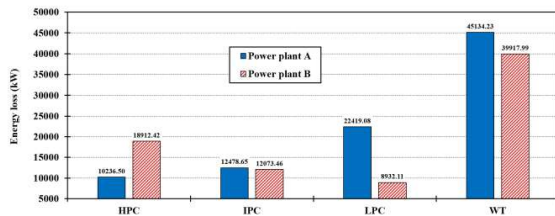


Fig. 4. Energy loss of the cylinders and whole turbine for a steam turbine from older power plant (A) and for a steam turbine from newer power plant (B)

In an older steam turbine, the highest energy loss of all cylinders can be seen in LPC, which is simultaneously the highest mechanical power producer, Fig. 3 and Fig. 4. In a newer steam turbine, the highest energy loss can be seen in HPC, which is not the dominant mechanical power producer, Fig. 3 and Fig. 4. Therefore, it is obvious that the same relations are not valid in both observed steam turbines.

Whole older steam turbine has higher energy loss (equal to 45.1 MW) in comparison to whole newer steam turbine (which energy loss is equal to 39.92 MW).

The energy efficiency of both observed steam turbines and their cylinders is presented in Fig. 5. The highest energy efficiency of all cylinders is calculated for HPC of an older steam turbine (equal to 79.82%), and for IPC of a newer steam turbine (equal to 89.46%). IPC and LPC of a newer steam turbine have notably higher energy efficiency in comparison to the same cylinders of an older steam turbine, while for the HPC this trend is opposite.

Whole newer turbine has notably higher energy efficiency in comparison to whole older turbine (83.52% in comparison to 77.28%). When comparing trends in energy loss and energy efficiency, Fig. 4 and Fig. 5, it is clear that older and newer steam turbine did not follow the same operation logic.

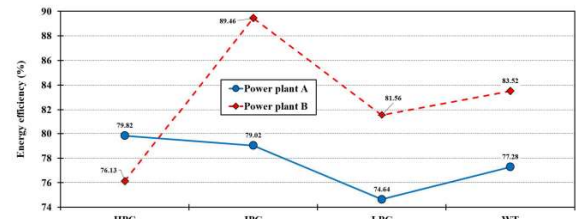


Fig. 5. Energy efficiency of the cylinders and whole turbine for a steam turbine from older power plant (A) and for a steam turbine from newer power plant (B)

Exergy analysis of any steam turbine or its cylinders considers different kind of losses in comparison to energy analysis. While energy analysis compares ideal and real expansion processes, exergy analysis considers losses between real expansion process and state of the ambient in which turbine operates.

Exergy loss of both observed turbines and their cylinders is shown in Fig. 6. Observation of the cylinders show that in an older steam turbine LPC has notably higher exergy loss than other cylinders, while in a newer steam turbine the highest energy loss can be seen in HPC (the same trend as obtained in an energy analysis).

Whole older steam turbine has notably higher cumulative exergy loss (equal to 32.7 MW) in comparison to a whole newer steam turbine which cumulative exergy loss is equal to around 26 MW.

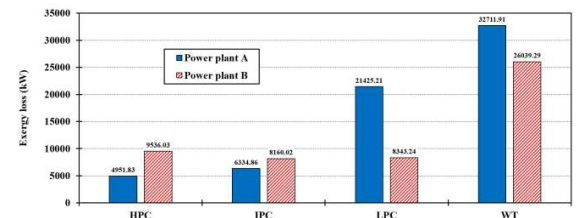


Fig. 6. Exergy loss of the cylinders and whole turbine for a steam turbine from older power plant (A) and for a steam turbine from newer power plant (B)

The same trends for the observed turbines and their cylinders obtained for the energy efficiency are also visible for exergy efficiency, Fig. 5 and Fig. 7.

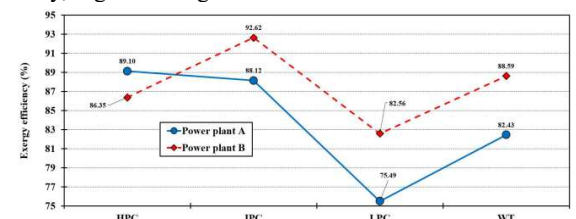


Fig. 7. Exergy efficiency of the cylinders and whole turbine for a steam turbine from older power plant (A) and for a steam turbine from newer power plant (B)

For a steam turbine from an older power plant, the cylinder with the highest exergy efficiency equal to 89.10% is HPC, while for a newer steam turbine, IPC has the highest exergy efficiency equal to 92.62%, Fig. 7. In an older steam turbine, LPC did not show the expected performance because its exergy efficiency is very low (equal to 75.49%), what is much lower than in any other cylinder from both observed turbines. As in energy efficiency, whole observed turbine from the newer power plant has much higher exergy efficiency in comparison to whole turbine from an older power plant (88.59% in comparison to 82.43%).

At the end of this analysis and comparison it is performed research related to the ambient temperature change influence on the exergy efficiency of both turbines. The ambient temperature is varied from 5 °C up to 45 °C in steps of 10 °C, while the ambient pressure remains constant and the same as at the base ambient state (equal to 1 bar).

From Fig. 8 can be concluded that the ambient temperature change sensitivity of the two observed steam turbines and their cylinders is reverse proportional to efficiencies (both energy and exergy). The whole older steam turbine is much more sensitive to the ambient temperature change than the whole newer steam turbine.

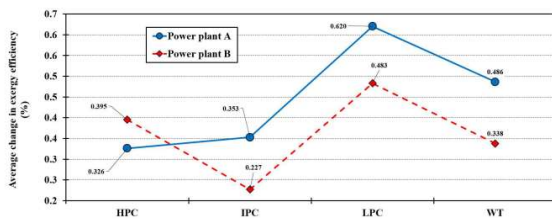


Fig. 8. Average change in exergy efficiency of the cylinders and whole turbine for a steam turbine from older power plant (A) and for a steam turbine from newer power plant (B)

6. Conclusions

In this paper are performed analysis and comparison of two similar steam turbines from conventional power plants. One turbine is from an older, while another turbine is from newer power plant. The most important obtained conclusions are:

- The dominant mechanical power producer in an older steam turbine is LPC (which produces mechanical power of almost 66 MW), while in a newer steam turbine the dominant mechanical power producer is IPC which produces power equal to 102.4 MW.
- Whole older steam turbine has a higher energy loss and higher exergy loss in comparison to the whole newer steam turbine.
- In an older steam turbine, LPC did not show the expected performance because its exergy efficiency is very low (equal to 75.49%), what is much lower than in any other cylinder from both observed turbines.
- Whole turbine from the newer power plant has much higher energy and exergy efficiencies in comparison to whole turbine from an older power plant.
- The ambient temperature change sensitivity of the two observed steam turbines and their cylinders is reverse proportional to efficiencies (both energy and exergy).

7. Acknowledgment

This research has been fully supported by the Croatian Science Foundation under the project IP-2022-10-2821.

8. References

[1] Tanuma, T. (Ed.). (2017). Advances in steam turbines for modern power plants. Woodhead Publishing.
[2] Elhelw, M., Al Dahma, K. S., & el Hamid Attia, A. (2019). Utilizing exergy analysis in studying the performance of steam power plant at two different operation mode. Applied Thermal Engineering, 150, 285-293. (doi:10.1016/j.applthermaleng.2019.01.003)
[3] Sutton, I. (2017). Plant design and operations. Gulf Professional Publishing

[4] Adibhatla, S., & Kaushik, S. C. (2014). Energy and exergy analysis of a super critical thermal power plant at various load conditions under constant and pure sliding pressure operation. Applied thermal engineering, 73(1), 51-65. (doi:10.1016/j.applthermaleng.2014.07.030)
[5] Andelić, N., Lorencin, I., Mrzljak, V., & Car, Z. (2024). On the application of symbolic regression in the energy sector: Estimation of combined cycle power plant electrical power output using genetic programming algorithm. Engineering applications of artificial intelligence, 133, 108213. (doi:10.1016/j.engappai.2024.108213)
[6] Mrzljak, V., Poljak, I., & Medica-Viola, V. (2017). Dual fuel consumption and efficiency of marine steam generators for the propulsion of LNG carrier. Applied Thermal Engineering, 119, 331-346. (doi:10.1016/j.applthermaleng.2017.03.078)
[7] Mrzljak, V., Poljak, I., & Mrakovčić, T. (2017). Energy and exergy analysis of the turbo-generators and steam turbine for the main feed water pump drive on LNG carrier. Energy conversion and management, 140, 307-323. (doi:10.1016/j.enconman.2017.03.007)
[8] Rosen, M. A. (2001). Energy-and exergy-based comparison of coal-fired and nuclear steam power plants. Exergy, An International Journal, 1(3), 180-192. (doi:10.1016/S1164-0235(01)00024-3)
[9] Mrzljak, V., Prpić-Oršić, J., & Poljak, I. (2018). Energy power losses and efficiency of low power steam turbine for the main feed water pump drive in the marine steam propulsion system. Pomorski zbornik, 54(1), 37-51. (doi:10.18048/2018.54.03)
[10] Medica-Viola, V., Pavković, B., & Mrzljak, V. (2018). Numerical model for on-condition monitoring of condenser in coal-fired power plants. International Journal of Heat and Mass Transfer, 117, 912-923. (doi:10.1016/j.ijheatmasstransfer.2017.10.047)
[11] Aljundi, I. H. (2009). Energy and exergy analysis of a steam power plant in Jordan. Applied thermal engineering, 29(2-3), 324-328. (doi:10.1016/j.applthermaleng.2008.02.029)
[12] Mrzljak, V., Lorencin, I., Andelić, N., & Car, Z. (2021). Thermodynamic Analysis of a Condensate Heating System from a Marine Steam Propulsion Plant with Steam Reheating. Journal of Marine Science and Application, 20(1), 117-127. (doi:10.1007/s11804-021-00191-5)
[13] Kanoğlu, M., Çengel, Y. A. & Dincer, I. (2012). Efficiency Evaluation of Energy Systems. Springer Briefs in Energy. (doi:10.1007/978-1-4614-2242-6)
[14] Gospić, I., Glavan, I., Poljak, I., & Mrzljak, V. (2021). Energy, economic and environmental effects of the marine diesel engine trigeneration energy systems. Journal of Marine Science and Engineering, 9(7), 773. (doi:10.3390/jmse9070773)
[15] Erdem, H. H., Akkaya, A. V., Cetin, B., Dagdas, A., Sevilgen, S. H., Sahin, B., ... & Atas, S. (2009). Comparative energetic and exergetic performance analyses for coal-fired thermal power plants in Turkey. International Journal of Thermal Sciences, 48(11), 2179-2186. (doi:10.1016/j.ijthermalsci.2009.03.007)
[16] Medica-Viola, V., Baressi Šegota, S., Mrzljak, V., & Štifić, D. (2020). Comparison of conventional and heat balance based energy analyses of steam turbine. Pomorstvo, 34(1), 74-85. (doi:10.31217/p.34.1.9)
[17] Mrzljak, V., Poljak, I., & Prpić-Oršić, J. (2019). Exergy analysis of the main propulsion steam turbine from marine propulsion plant. Brodogradnja: Teorija i praksa brodogradnje i pomorske tehnike, 70(1), 59-77. (doi:10.21278/brod70105)
[18] Kopac, M., & Hilalci, A. (2007). Effect of ambient temperature on the efficiency of the regenerative and reheat Çatalağzı power plant in Turkey. Applied Thermal Engineering, 27(8-9), 1377-1385. (doi:10.1016/j.applthermaleng.2006.10.029)
[19] Jahangiri, A., & Ameri, M. (2020). Interaction effects of natural draft dry cooling tower (NDDCT) performance and 4E (energy, exergy, economic and environmental) analysis of steam power plant under different climatic conditions. Sustainable Energy Technologies and Assessments, 37, 100599. (doi:10.1016/j.seta.2019.100599)
[20] Lemmon, E. W., Huber, M. L., & McLinden, M. O. (2010). NIST Standard Reference Database 23, Reference Fluid Thermodynamic and Transport Properties (REFPROP), version 9.0, National Institute of Standards and Technology. R1234yf. fld file dated December, 22, 2010.

Determination Of Physico-Chemical Parameters Of Hydrocarbon Gas Based On Field Data.

Lusjen Ismaili

Specialist in the sector of development programs in the oil field

Ministry of Infrastructure and Energy, Tiranë, Albania

ismaililusjen1@gmail.com

Abstract: The fluids that are present in the underground reservoirs of oil and gas, both in the initial conditions and in the exploitation conditions of the reservoir, experience different phase behavior. All these are accompanied by different physico-chemical parameters, the determination of which plays an important role in the hydrodynamic study of the well or the reservoir as a whole. The fluids released from the formation change over time due to the change in the phase state of the fluids, their material and energy balance. In this study, based on the field data obtained during the exploitation of the oil and gas bearing bed, the physico-chemical parameters of the gas were determined based on the correlations derived from the various experimental studies carried out in the world.

KEYWORDS: PRESSURE, GAS, TEMPERATURE, Z-FACTOR, DENSITY, COMPRESSIBILITY.

1. Introduction

From a technical point of view, based on certain values of pressure and temperature as well as phase changes that occur as a result of different conditions that are created during the exploitation of the reservoir, the relevant pressure-temperature and pressure-volume diagrams are built that make it possible to determine the type of reservoir and the behavior of the fluids with the characteristic physical and chemical parameters [1]. During the exploitation of the oil-gas bearing layer, both the pressure and the temperature change, which lead to changes in the physico-chemical parameters of the fluids, including the molecular composition, density, viscosity, etc [2]. For many purposes and engineering calculations, both for liquids and gases, some assumptions are made to better approximate their behavior in the layer conditions. For example, the behavior of real gases can be approximated to the behavior of ideal gases by

using a deviation factor called the compressibility factor [3,4]. Hydrocarbon gases themselves contain different chemical elements, depending on their content it is possible to classify the gases into light gases, heavy gases and acid or neutral gases. Physical and chemical properties of gases, such as: isothermal gas compressibility coefficient, specific volume, density, viscosity, gas formation volume factor, gas expansion factor, apparent molecular weight, specific gravity, compressibility factor, are calculated both from direct measurements performed in the laboratory and from prediction (general mathematical expressions) or corresponding correlations obtained from the analysis of various experiments performed in relation to real gases. [5,6,7].

2. Methodology

In this paper, the initial pressure of the layer was measured and result to be 368 atm and the temperature result to be 40 °C. Based on the data obtained in the field and concretized and calculated in tables 1 and 2, we will calculate different parameters, both physical and chemical, of the fluid taken into consideration. Calculations of the physico-chemical parameters for the considered fluid (hydrocarbon gas) are made not only for the initial pressure of the reservoir, but also for values different from the initial pressure of the reservoir, to demonstrate the behavior of the fluid with the change of pressure and the representation its graph.

Table 1-Composition of hydrocarbon gas.

Component	Mole fraction of component	Critical temperature °R T_{ci}	Critical pressure P_{ci}	Molecular weight
C ₁	0.94	343.04	667.8	16.04

C ₂	0.02	549.76	707.8	30.07
C ₃	0.005	665.68	616.3	44.11
n-C ₄	0.004	765.32	550.7	58.1
n-C ₅	0.003	470.4	488.6	72.2
CO ₂	0.007	547.6	1071	44.01
H ₂ S	0.008	672.4	1306	34.08
N ₂	0.013	227.3	493	28.016

Table 2-Calculation of pseudocritical pressure and temperature.

Component	Pseudocritical pressure $\gamma_i * P_{ci}$	Pseudocritical temperature $\gamma_i * T_{ci}$
C ₁	627.732	322.457
C ₂	14.156	10.995
C ₃	3.081	3.328
n-C ₄	2.202	3.061
n-C ₅	1.465	1.411
CO ₂	7.497	3.833
H ₂ S	10.448	5.379
N ₂	6.409	2.954
	$\Sigma=672.99$ psi	$\Sigma=353,418$ °R

3. Results and Discussion.

Based on the values presented in table 1 and 2, below is presented the method followed for determining the z-factor in the case of the initial pressure of the layer and then based on this method the values of the z-factor are determined for pressure values different from that of the initial pressure of the layer and their graphic presentation was built.

For P=368 atm T=40°C

Converting the pressure to the psi unit and the temperature to °R, we get the values:

$$P_i = 375 * 14.696 = 5510.99 \text{ psi}$$

$$°F = 1.8 T°C + 32 = 1.8 * 40 + 32 = 104$$

$$°R = °F + 460 = 104 + 460 = 564$$

Second, we calculate the pseudo-critical properties by making the Carr-Kobayashi-Burrows corrections:

$$T_{pc}^* = T_{pc} - 80 * \gamma_{CO_2} + 130 * \gamma_{H_2S} - 250 * \gamma_{N_2}$$

$$P_{pc}^* = P_{pc} + 440 * \gamma_{CO_2} + 600 * \gamma_{H_2S} - 17 * \gamma_{N_2}$$

$$T_{pc}^* = 353.418 - 80(0.007) + 130(0.008) - 250(0.013)$$

$$T_{pc}^* = 350.650$$

$$P_{pc}^* = 672.99 + 440(0.007) + 600(0.008) - 170(0.013)$$

$$P_{pc}^* = 678.662.$$

Thirdly, the pseudo-reduced pressure and temperature are calculated as following:

Figure 1-Graphical Presentation $z=f(p)$

$$P_{pr} = \frac{P}{P_{pc}} = \frac{5409.6}{678.66} = 7.97$$

$$T_{pr} = \frac{T}{T_{pc}} = \frac{564}{350.648} = 1.608$$

The fourth z-factor is calculated from the Standing and Katz chart: **$Z=0.99$**

Based on the method and equations for determination of the z-factor for the initial pressure of the layer, we determine the z-factor for the different pressure values, specifically; 20 Mpa, 15 Mpa, 10 Mpa, 5 Mpa, 2 Mpa and 1 Mpa for the same temperature $T = 40^\circ\text{C}$. With the values obtained from the performed calculations, we construct the graph of the z-factor versus pressure.

20 Mpa $\rightarrow Z = 0.822$; 15 Mpa $\rightarrow Z = 0.819$; 10 Mpa $\rightarrow Z = 0.854$; 5 Mpa $\rightarrow Z = 0.958$; 2 Mpa $\rightarrow Z = 0.919$; 1 Mpa $\rightarrow Z = 0.981$.

To determine the gas formation volume factor both for the value of the initial pressure of the layer and for the different values of the pressures, we use the equation as following:

For initial pressure:

$$P = 5409.6 \text{ psi} \quad T = 564^\circ\text{R} \quad z = 0.919$$

$$B_g = 0.02827 * \frac{z * T}{p} = 0.02827 * \frac{0.919 * 564}{5409.6} = 2.9179 \times 10^{-3} \text{ ft}^3/\text{scft}$$

For $P = 20 \text{ Mpa}$

$$P = 2901.554 \text{ psi} \quad T = 564^\circ\text{R} \quad z = 0.822$$

$$B_g = 0.02827 * \frac{z * T}{p} = 0.02827 * \frac{0.822 * 564}{2901.554} = 4.5169 \times 10^{-3} \text{ ft}^3/\text{scft}$$

For $P = 15 \text{ Mpa}$

$$P = 2176.16 \text{ psi} \quad T = 564^\circ\text{R} \quad z = 0.819$$

$$B_g = 0.02827 * \frac{z * T}{p} = 0.02827 * \frac{0.819 * 564}{2176.16} = 6.0062 \times 10^{-3} \text{ ft}^3/\text{scft}$$

For $P = 10 \text{ Mpa}$

$$P = 1450.77 \text{ psi} \quad T = 564^\circ\text{R} \quad z = 0.854$$

$$B_g = 0.02827 * \frac{z * T}{p} = 0.02827 * \frac{0.854 * 564}{1450.77} = 9.385 \times 10^{-3} \text{ ft}^3/\text{scft}$$

For $P = 5 \text{ Mpa}$

$$P = 725.388 \text{ psi} \quad T = 564^\circ\text{R} \quad z = 0.919$$

$$B_g = 0.02827 * \frac{z * T}{p} = 0.02827 * \frac{0.919 * 564}{725.388} = 20.199 \times 10^{-3} \text{ ft}^3/\text{scft}$$

For $P = 2 \text{ Mpa}$

$$P = 290.550 \text{ psi} \quad T = 564^\circ\text{R} \quad z = 0.971$$

$$B_g = 0.02827 * \frac{z * T}{p} = 0.02827 * \frac{0.971 * 564}{290.550} = 53.28 \times 10^{-3} \text{ ft}^3/\text{scft}$$

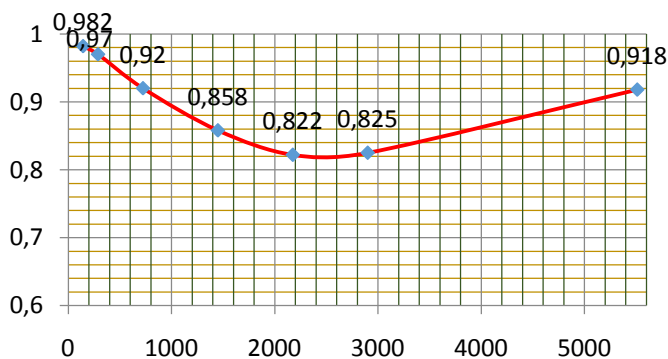
For $P = 1 \text{ Mpa}$

$$P = 145.077 \text{ psi} \quad T = 564^\circ\text{R} \quad z = 0.981$$

$$B_g = 0.02827 * \frac{z * T}{p} = 0.02827 * \frac{0.981 * 564}{145.077} = 107.81 \times 10^{-3} \text{ ft}^3/\text{scft}$$

Figure 2-Graphical Presentation $B_g = f(p)$

Another parameter that will be determined is the gas density and



gas compressibility coefficient, which are calculated as following:

$$M_a = \sum_{i=1}^n \gamma_i * M_i \rightarrow M_a = 17.291$$

$$P = 5409.6 \text{ psi and } T = 564^\circ\text{R}$$

$$T_{pc}^* = 350.648 \rightarrow T_{pr} = 1.608$$

$$P_{pc}^* = 678.66 \rightarrow P_{pr} = 7.97$$

$$Z = 0.99$$

$$\rho_g = \frac{P * M_a}{Z * R * T}$$

$$\rho_g = \frac{5409.6 * 17.29}{0.99 * 10.73 * 564} = \text{lb}/\text{ft}^3$$

$$\Delta z = z_2 - z_1 = 0.99 - 0.97 = 0.02$$

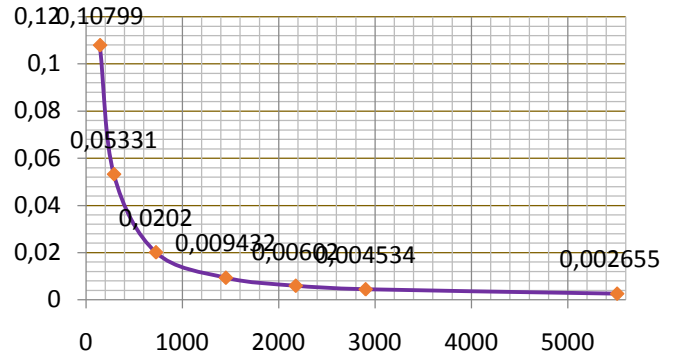
$$\Delta P_r = P_{r2} - P_{r1} = 7.97 - 7.5 = 0.47$$

$$\left[\frac{\partial Z}{\partial (P_{pr})} \right]_{T_{pr}} = 0.042$$

$$C_{pr} = \frac{1}{P_{pr} * P_{pc}} - \frac{1}{Z} * \left[\frac{\partial Z}{\partial (P_{pr} * P_{pc})} \right]_{T_{pr}}$$

$$C_{pr} = \frac{1}{P_{pr}} - \frac{1}{Z} * \left[\frac{\partial Z}{\partial (P_{pr})} \right]_{T_{pr}}$$

$$C_{pr} = \frac{1}{7.97} - \frac{1}{0.99} * [0.042] = 0.083030$$



$$C_g = \frac{C_{pr}}{P_{pc}}$$

$$C_g = \frac{0.083030}{678.66} = 0.000122 \text{ psi}^{-1}$$

The pseudo-critical properties presented above, which are expressed through the parameters P_{pc} and T_{pc} , do not in themselves represent critical properties of the gas mixture, but are parameters that make possible the correlative relationship which, together with the graphs taken into consideration, reach the accuracy of designated for determining the respective properties of hydrocarbon gases. From the formulas and calculations performed, it can be judged on the dependence of the parameters defined above on temperature and pressure [5,7]. As the pressure increases, the gas density and, compressibility factor increases, but the average free path of molecules decreases, while the speed remains unchanged. Another important parameter that must be taken into consideration is the viscosity of gases [8,9]. As the temperature increases, the viscosity of the gas decreases therefore, at high pressures, the viscosity of gases changes as a function of temperature so as viscosity of liquids [8,9,10]. Gases with higher molecular weight usually have higher viscosity. While in relation to the increase in pressure, the density of the gas increases, but the average free path of molecules decreases, while the speed remains unchanged [7,10]. So as the pressure increases, the dynamic viscosity of the gas remains practically unchanged.

4. Conclusion

In this study the gas from the gas cap of a gas-condensate field located in Albania was taken into consideration, determining its properties through the relevant correlations and the use of different graphs. After performing various measurements in the gas-condensate field in relation to the initial pressure of the layer and the average temperature of the reservoir, the composition of the gas sample from gas cap taken into consideration was analyzed. From the calculation and analysis of the above parameters for the fluid taken into consideration (hydrocarbon gas), we can say that the phase behavior of the gas is related and directly affected by the change in pressure and temperature. The correlation and accuracy of the calculations performed are dependent and influenced by the dimensionless pseudocritical parameters used in relation to

pressure and temperature, as well as the graphs that express the dependence between them.

5 . References

- [1] Abdus Satter, Ghulam M. Iqbal Reservoir Engineering The Fundamentals, Simulation, and Management of Conventional and Unconventional Recoveries 2016, Pages 107-115
- [2] James G. Speight PhD, DSc Introduction to Enhanced Recovery Methods for Heavy Oil and Tar Sands (Second Edition) 2016, Pages 123-175
- [3] Ronald E. Terry, J. Brandon Rogers Applied petroleum reservoir engineering Third Edition, 2015 Pearson Education, Inc.
- [4] Fundamentals of Petroleum Reservoir Engineering, J.-R. Ursin & A. B. Zolotukhin Stavanger, 1997
- [5] Huinong Zhuang, ... Xiaohua Liu, in Dynamic Well Testing in Petroleum Exploration and Development (Second Edition) 2020, Pages 491-673
- [6] Tarek Ahmed, Paul D. McKinney Advanced Reservoir Engineering Gulf Professional Publishing is an imprint of Elsevier 200 Wheeler Road, Burlington, MA 01803, USA Linacre House, Jordan Hill, Oxford OX2 8DP, UK
- [7] L.P.Dake fundamentals of reservoir engineering ELSEVIER, Amsterdam London New York Tokyo, 1978 ELSEVIER SCIENCE B.V
- [8] Curtis H. Whiston Petroleum Reservoir Fluid Properties Available from:
<http://www.ipt.ntnu.no/~curtis/courses/PVT-Flow/2016-TPG4145/Handouts/Petroleum-Reservoir-Fluid-Properties-Whitson.pdf>
- [9] Ahmed Hamza, Ibnel waleed A.Hussein, Mohamed Mahmoud Developments in Petroleum Science Volume 78 , 2023, Pages 1-19 Available from:
<https://www.sciencedirect.com/science/article/abs/pii/B978032399285500003X>
- [10] Tarek Ahmed Reservoir Engineering Handbook Fifth Edition, 2019 Elsevier Inc Gulf Professional Publishing is an imprint of Elsevier 50 Hampshire Street, 5th Floor, Cambridge, MA 02139, United States The Boulevard, Langford Lane, Kidlington, Oxford, OX5 1GB, United Kingdom.

Modeling of Shredding Blade for Nonwoven Waste Fabric

Enes Bitigen^{1,2}, Ali H. Nazik^{1,2}, Tahsin Topbaşoğlu¹, Onur Çimen¹, İ.Etem Saklakoğlu^{1,2}
KANSAN R&D Center, Izmir, Türkiye¹
Ege University, Department of Mechanical Engineering, Izmir, Türkiye²
enesbitigen@kansanmak.com

Abstract: In this study, cutter blades were designed to shred nonwoven waste fabrics by being positioned on an existing shaft. In this context, the design was carried out by considering the shear stress and density of the material to be shredded. During the design process, the total deformation conditions on the cutting surface were examined, and the stress concentration regions were identified using the von Mises approach to determine the necessary mechanical properties of the cutter blade. At this stage, the most suitable cutting tool material was selected. To ensure the torque from the motor is evenly distributed to the cutting edges and to meet the requirements of the material to be cut/shredded as well as the targeted machine capacity, various tool geometries were created and designed. In this context, analyses were performed to determine the effect of the selected geometries on the load distribution on the cutting edges, and the optimal tool geometry was decided.

KEYWORDS: CUTTER BLADE DESIGN, NONWOVEN WASTE FABRIC, SHEAR STRESS, BLADE GEOMETRY, CUTTING PERFORMANCE, HEXAGONAL HUB CONNECTION, CUTTING EDGE OPTIMIZATION.

1. Introduction

Nonwoven fabrics are widely utilized in the production of various products, including wet wipes, cleaning cloths, and floor cloths. KANSAN has been manufacturing wet wipe machines for many years, distributing them globally. A significant amount of nonwoven waste is generated by the companies using these machines, which is currently treated as waste, leading to additional disposal costs.

The primary aim of this study is to develop a cutting and shredding tool capable of converting nonwoven waste, produced during the manufacturing of cleaning products such as wet wipes, into reusable raw material. This tool would allow companies to reduce disposal costs and contribute to sustainable resource management by repurposing production waste.

2. Method

The design process began with the use of SolidWorks software. Initially, the blade geometry was created in two dimensions. During this phase, an optimal design was established to ensure that the motor's torque was evenly distributed across all cutting edges. Additionally, geometric adjustments were made at the shaft-blade connection to increase the blades' resistance to the torsional forces acting on the shaft. In this context, a hexagonal hub connection was selected.

The primary factor in determining the blade geometry was the reaction force generated by the material during the shredding process. Based on this, the number of cutting edges and the cutting edge area were defined. An average cutting resistance of 3 N/mm was used as a reference for nonwoven fabrics, and the cutting edge design was tailored to counter this resistance.

In addition to cutting resistance, the target shredding capacity and the system's RPM were also decisive in calculating the number of cutting edges. Consequently, the blade geometry was shaped to meet these parameters.

The thickness and diameter of the blade were determined based on the cutting force applied to the cutting edge area, and the depth and width of the cutting edges were defined accordingly. These dimensional parameters were carefully considered when performing the necessary calculations.

Another important feature of the blade is the cutting angle, defined as the angle between the cutting edges and the main structure of the blade. A larger cutting angle provides a wider gripping area, allowing for improved cutting performance under higher shredding forces [1]. Figure 1 shows the configuration of the pre-designed blades. The set on the right includes blades with four cutting edges [2], while the set on the left has blades with three cutting edges [3,4,5]

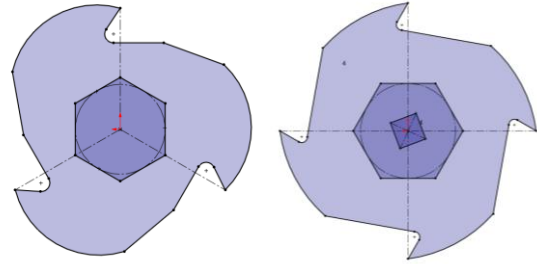


Figure 1: Basic design of cutting edges

3. Materials for Cutter Blade

A wide range of blade materials (from alloys to stainless steels) is available for shredding process. Table 1 specifies the mechanical properties of some selected blade materials.

Table 1: Mechanical properties of selected blade materials

	Cold work tool steel 1.2379 (X153CrMoV 12)	316 Stainless steel (1.4401)	High carbon alloy steel 1.7225 (42CrMo4)
Abrasive hardness	55 - 62 HRC	25-30 HRC	28-32HRC
Tensile strength Rm [MPa]	850 - 1000	515	655-1030
Yield strength Rm [MPa]	450-600	205	415-690
Wear resistance	Very High	Medium	Medium
Corrosion resistance	Medium	High	Low
Modulus of elasticity [GPa]	210	193	190-210
Coefficient of thermal expansion [µm/m°C]	10.4	16	12.2
Density [g/cm³]	7.7	8.0	7.85

The blade material selected for the study is 1.2379 (X153CrMoV12) steel. This cold work tool steel has excellent mechanical properties for the necessary mechanical values. 1.2379 steel is extremely resistant to wear due to the presence of vanadium.

It is classified as semi-stainless due to the presence of 13% chromium. 1.2379 has high hardness and is a tough material. For this reason, it is durable for a long time under abrasive conditions. The high carbide resistance of the material increases its resistance to unwanted solid particle accumulation and abrasive effects on the surface. This durability enhances the material's service life and maintains surface quality. This material is preferred in various molds, knives, cutting tools, drilling tools, and forming tools. The analysis and calculations conducted have shown that the selected 1.2379 steel possesses the necessary mechanical properties.

4. Static Load Analysis of the Cutter Blade

Assuming the cutter blade is in a static state, the stresses it experiences were simulated in a computer environment. The purpose of this simulation is to verify the suitability of the geometric calculations and material type for the intended operation.

In the simulations, the amount of deformation on the cutting edges, equivalent stress, and normal stress values were examined. The consistency of these values was first evaluated, and then compared with values obtained from existing studies. Table2 presents values obtained from various studies.

Table 2: Values from Various Studies [5,6,7]

	Ravi (2018)	Akash (2019)	Kumaran (2020)
Material of blade	Tool Steel with Chromium or Nickel coating	Mild Steel	Cast iron blade with Nickel coating
Blade Thickness (mm)	5	7	20
Diameter (mm)	100	184	150
Cutting Edge	2	4	3
Max. Von Mises Stress (Pa)	2.47×10^6	360.05×10^6	164×10^6
Elastic Shear Strain	1.24×10^{-5}	4.68×10^{-3}	1.02×10^{-5}
Deformation	4.03×10^{-6}	3.07×10^{-4}	3.78×10^{-5}

The suitability of the design can be evaluated based on the simulation results. Adjustments to the design or changes in material selection can be made as necessary, guided by these results and their comparisons. [8]

5. Results

The simulation results of the cutter blade designed in this study are presented in Table 3. The findings demonstrate consistency and align closely with existing studies.

When determining the input parameters for the analysis, the primary factors influencing the simulation results are the shear stress and dimensions of the material to be shredded. Higher shear stress in the material results in increased stress on the cutting edges. Consequently, it is imperative to design the blade in accordance with the specific properties of the material to be processed.

Finite element analyses confirmed that the geometry of the cutting blade satisfies the operational requirements. The analyses also indicated that the stresses on the cutting edges are uniformly distributed along the shaft.

Figure 2 a-b-c shows the simulation of the mechanical load distributions and deformation in the tool . Table-3 presents the values obtained from the simulation of the cutter blade designed in this study. The results demonstrated consistency and showed alignment with findings from previous studies.

Table 3: Stress and Deformation Values of the Cutter Blade Under Static Load

Material of blade	Steel 1.2379 (X153CrMoV12)
Blade Thickness (mm)	5
Diameter (mm)	110
Cutting Edge	4
Max. Von Mises Stress (Pa)	2.39×10^6
Elastic Shear Strain	1.19×10^{-5}
Deformation	5.01×10^{-4}

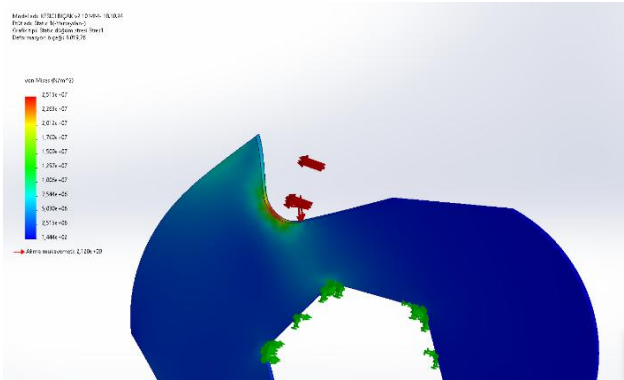


Fig. 2a: Static Stress (Von-Mises N/m^2) distribution on a single cutting edge.

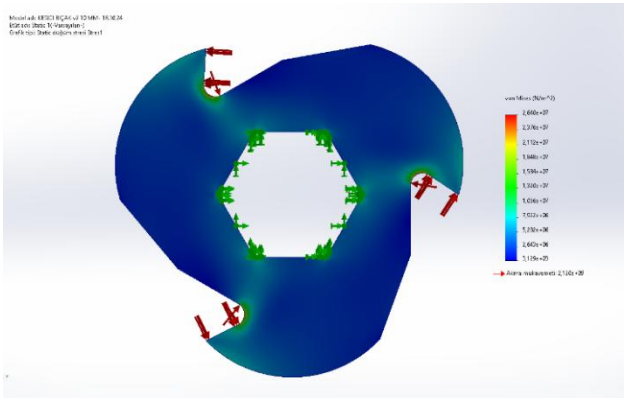


Fig. 2b: Static Stress (Von-Mises N/m^2) distribution for three cutting edges

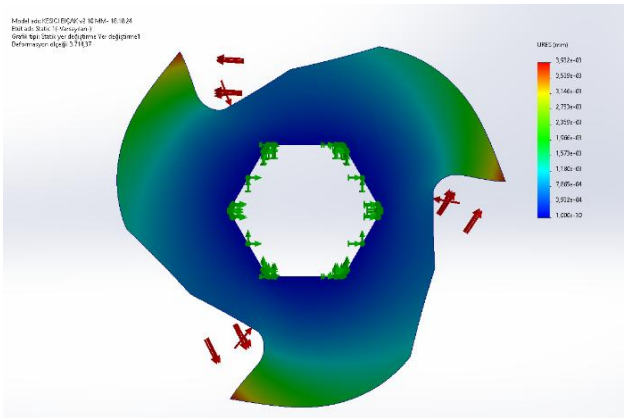


Fig. 2c: Deformations (mm)

6. Conclusion

In this study, a cutting-shredding design was developed for processing waste fabrics. The outputs obtained from the completed work can be summarized as follows.

In determining the input parameters for the analysis, the shear stress and dimensions of the material to be shredded are key factors that influence the simulation results. Higher shear stress in the shredded material will increase the stress exerted on the cutting edges. Thus, it is essential to design the blade according to the specific properties of the material being processed.

7. References

1. *Engineering and Operations Management* (pp. 1-10). Paris, France.
2. Tegegne, A., Tsegaye, A., Ambaye, E., & Mebrhatu, R. (2019). Development of dual shaft multi blade waste plastic shredder for recycling purpose. *International Journal of Research and Science Innovation (IJRSI)*, 6.
3. Ekman, R. (2018). *Development of a plastic shredder* (Master's thesis, Lund University, Sweden).
4. Biddinika, M. K., Syamsiro, M., Hadiyanto, A. N., Mufrodi, Z., & Takahashi, F. (2017). Technology for public outreach of fuel oil production from municipal plastic wastes. *Energy Procedia*, 142, 2797-2801. <https://doi.org/10.1016/j.egypro.2017.12.411>
5. Yepes, C. P., Pelegrina, R. M. A., & Pertuz, M. G. J. (2018). Analysis by means of the finite element method of the blades of a PET shredder machine with variation of material and geometry. *Contemporary Engineering Sciences*, 11(83).
6. Ravi, S. (2018). Utilization of upgraded shredder blade and recycling the waste plastic and rubber tyre. In *Proceedings of the International Conference on Industrial*
7. Akash, B. P., Christina, S. D. K., & Manoj. (2019). Plastic waste management by mechanical shredder machine. *International Journal of Advanced Research in Innovative Ideas in Engineering (IJARIIEE)*, 5(2), 3218-3223.
8. Dattatraya, R. P., & Bhalgat, S. M. (2020). Cutter blade design for shredder machine. *International Journal of Scientific Research Publications*, 10(06), 1022-1027. <https://doi.org/10.29322/IJSRP.10.06.2020.p10294>

Mathematical modeling of aluminum alloys

Adelina Miteva, Margarita Dimitrova

Space Research and Technology Institute, Bulgarian Academy of Sciences, Sofia, Republic of Bulgaria

ad.miteva@gmail.com, m.dimitrova@space.bas.bg

Abstract: Aluminum alloys are critical in industries such as aerospace and automotive due to their lightweight, strength, and corrosion resistance. Optimizing their properties is challenging and benefits from advanced predictive tools. This paper explores the use of mathematical modeling in understanding and designing aluminum alloys. Techniques like thermodynamic modeling (e.g., CALPHAD), phase transformation kinetics, and mechanical property simulations are reviewed. Computational methods, including finite element analysis and machine learning, are highlighted for their roles in alloy design and manufacturing, such as casting and additive manufacturing. Comparisons between model predictions and experimental results demonstrate accuracy and limitations. Applications in optimizing material properties and improving manufacturing processes are discussed. By accelerating alloy development and enabling tailored properties, mathematical modeling emerges as a transformative tool, advancing aluminum alloy research and driving innovation across industries.

Keywords: ALUMINUM ALLOYS, MATHEMATICAL MODELING, THERMODYNAMIC MODELING, PHASE TRANSFORMATIONS, MECHANICAL PROPERTIES, CALPHAD, FINITE ELEMENT ANALYSIS, MACHINE LEARNING, ALLOY DESIGN, ADDITIVE MANUFACTURING

1. Introduction

Aluminum alloys [1] are among the most widely used materials in modern industries due to their remarkable combination of properties, including lightweight, high strength, corrosion resistance, and thermal conductivity. In the aerospace sector, aluminum alloys are critical for reducing aircraft weight while maintaining structural integrity. Similarly, in the automotive industry, they contribute to fuel efficiency and emission reduction through lightweighting. In construction, their durability and corrosion resistance make them ideal for structural and architectural applications.

Despite these advantages, optimizing the properties of aluminum alloys to meet diverse performance requirements remains a significant challenge. Factors such as strength, ductility, corrosion resistance, and thermal stability must often be balanced, making alloy development a complex process. Furthermore, the introduction of advanced manufacturing techniques, such as additive manufacturing and high-pressure die casting, necessitates the design of alloys that perform well under specific processing conditions. Addressing these challenges requires an in-depth understanding of the relationships between alloy composition, microstructure, and properties.

Mathematical modeling has emerged as a transformative tool for understanding and optimizing aluminum alloys. By providing a framework for predicting material behavior based on composition, thermodynamics, and processing conditions, mathematical models enable researchers and engineers to streamline the design of new alloys. This predictive capability reduces reliance on traditional trial-and-error methods, which are time-consuming and resource-intensive.

Models such as CALPHAD [2-4] allow for the accurate prediction of phase diagrams and equilibrium properties, enabling the selection of alloying elements that enhance performance. Kinetic models [5] help to simulate microstructural evolution during manufacturing, while mechanical property models [5-9] predict stress-strain behavior and failure mechanisms under various loading conditions. By integrating these tools, researchers can design alloys tailored to specific applications, improving efficiency and reducing development costs.

This study aims to provide a comprehensive overview of mathematical modeling techniques for aluminum alloys, focusing on their theoretical foundations and practical applications. It seeks to outline key modeling methods, including thermodynamic, kinetic, and mechanical models, and demonstrate how these approaches can be applied to optimize alloy properties and manufacturing processes.

Additionally, this article highlights the applications of mathematical modeling in understanding and improving the performance of aluminum alloys. By showcasing examples of successful alloy design and identifying areas for future research, this work underscores the critical role of mathematical modeling in

advancing aluminum alloy technology and driving innovation across industries.

2. Fundamentals of Mathematical Modeling in Alloy Design

Thermodynamics forms the foundation for understanding the behavior of aluminum alloys by describing the equilibrium states and phase transformations within an alloy system. Phase diagrams are critical tools in alloy design, providing insights into phase stability, melting points, solubility limits, and the interactions between alloying elements. These diagrams guide the selection of compositions that yield desired properties such as strength, ductility, and corrosion resistance.

One of the most widely used tools for thermodynamic modeling is the CALPHAD (CALculation of PHase Diagrams) approach. CALPHAD enables the prediction of phase stability and equilibrium compositions based on thermodynamic principles and experimental data. By constructing multi-component phase diagrams, CALPHAD helps identify optimal alloy compositions and processing conditions. For aluminum alloys, this is particularly useful in designing systems with complex combinations of elements, such as Al-Mg-Si, Al-Zn-Mg, and Al-Cu alloys. These predictions are invaluable for ensuring that alloys meet performance requirements while minimizing the need for extensive experimental testing.

While thermodynamics predicts equilibrium states, the kinetics of phase transformations describe how these states are achieved during manufacturing and use. Kinetic modeling focuses on diffusion-driven processes, nucleation, and growth mechanisms that dictate microstructural evolution in aluminum alloys.

Diffusion models quantify the transport of atoms within an alloy, which governs phase transformations, precipitation, and homogenization. Mathematical formulations such as Fick's laws of diffusion and numerical simulations are used to predict the rate and extent of these processes under varying thermal and mechanical conditions.

Nucleation and growth models are equally important for understanding the formation of secondary phases, which significantly impact mechanical properties. For example, precipitation hardening in aluminum alloys, such as the Al-Mg-Si and Al-Cu systems, depends on the controlled formation of finely dispersed precipitates. Accurate modeling of these transformations helps optimize heat treatment schedules, ensuring the desired balance of strength and ductility.

The mechanical performance of aluminum alloys is a critical factor in their application. Mathematical models that describe stress-strain behavior, deformation mechanisms, and failure modes provide valuable insights into alloy performance under various loading conditions.

Stress-strain behavior is often modeled using constitutive equations, such as those based on elasticity, plasticity, and

viscoelasticity theories. These models enable the prediction of how an alloy responds to mechanical loads, including elastic deformation, yielding, and strain hardening.

Fatigue, creep, and fracture models are essential for assessing the durability of aluminum alloys in demanding environments. Fatigue modeling, for instance, involves understanding crack initiation and propagation under cyclic loading, which is vital for aerospace and automotive applications. Similarly, creep models predict time-dependent deformation under high temperatures, and fracture mechanics helps assess the resistance of alloys to crack growth. Together, these models provide a comprehensive framework for designing aluminum alloys that meet stringent performance criteria.

By integrating thermodynamics, kinetics, and mechanical modeling, researchers and engineers can gain a holistic understanding of aluminum alloys, enabling the design of materials with tailored properties for specific applications.

3. Methodology

Computational techniques form the backbone of mathematical modeling for aluminum alloys. A variety of software tools and algorithms are employed to predict alloy behavior, optimize compositions, and simulate manufacturing processes.

CALPHAD-based tools, such as Thermo-Calc and Pandat, are widely used to calculate phase diagrams, predict phase stability, and assess equilibrium properties. These tools utilize thermodynamic databases to provide accurate predictions for multi-component aluminum alloy systems. Finite Element Analysis (FEA) software, like ANSYS or Abaqus, is critical for simulating mechanical behavior under different loading conditions, offering insights into stress distribution, deformation, and failure mechanisms.

Machine learning approaches are increasingly integrated into the modeling process to predict alloy properties and optimize compositions. These techniques leverage large datasets to identify patterns and relationships between composition, microstructure, and properties. Machine learning algorithms, such as neural networks and decision trees, are particularly useful for exploring vast design spaces and generating predictions for properties like strength, ductility, and corrosion resistance.

The development of predictive models for aluminum alloys involves several key steps and requires high-quality input data.

Input Data Requirements: Accurate input data is crucial for reliable model predictions. This includes alloy compositions, thermophysical properties (e.g., thermal conductivity, heat capacity), and material behavior data (e.g., stress-strain curves, creep rates). Experimental datasets and thermodynamic databases provide much of this information, supplemented by data from prior simulations.

Steps in Model Development:

- **Data Collection and Preprocessing:** Gather and validate input data, ensuring consistency and completeness.
- **Model Formulation:** Define the mathematical framework, such as thermodynamic equations, kinetic models, or machine learning architectures.
- **Simulation and Calibration:** Run simulations using computational tools and adjust model parameters to align with known behaviors.
- **Testing and Validation:** Compare predictions with experimental results to assess model accuracy. Refine the model based on discrepancies.
- **Optimization:** Use the validated model to explore the design space, identify optimal alloy compositions, and predict performance under different conditions.

Experimental validation is essential for ensuring the reliability of mathematical models. Laboratory techniques are employed to test predictions and provide feedback for model refinement.

Microstructure Analysis: Techniques like scanning electron microscopy (SEM), transmission electron microscopy (TEM), and X-ray diffraction (XRD) are used to examine the phases and microstructural features predicted by thermodynamic and kinetic

models. For instance, precipitation patterns and grain structures can be compared against model outputs to verify accuracy.

Mechanical Testing: Mechanical properties such as tensile strength, hardness, fatigue resistance, and creep behavior are evaluated through standard tests. These results are compared with predictions from mechanical behavior models, ensuring that the simulations accurately represent real-world performance.

Integration of Experimental Data: Experimental results are fed back into the modeling process to improve predictions. For example, discrepancies between predicted and observed phase compositions can be used to refine thermodynamic databases, while variations in mechanical behavior can guide the adjustment of constitutive equations. This iterative process strengthens the model's reliability and expands its applicability.

By combining computational techniques with rigorous experimental validation, this methodology ensures robust and accurate modeling of aluminum alloys, paving the way for more efficient alloy development and optimization.

4. Applications of Mathematical Models

Mathematical models play a crucial role in the design and optimization of aluminum alloys, enabling the tailoring of compositions to meet specific performance requirements. Through the use of thermodynamic and kinetic models, alloy compositions can be optimized for properties such as strength, corrosion resistance, and thermal stability. These models allow researchers to predict phase stability and microstructural evolution, guiding the selection of appropriate alloying elements and their concentrations to achieve desired characteristics.

One of the key applications of modeling in alloy design is the development of high-strength, lightweight aluminum alloys. For example, models can predict the optimal amounts of elements like magnesium (Mg), silicon (Si), and zinc (Zn) for achieving the desired combination of tensile strength and ductility, which is critical for industries such as aerospace and automotive. By simulating the effects of different alloying elements and heat treatment processes, researchers can accelerate the discovery of alloys with improved mechanical properties without the need for extensive experimental trials. These predictions help reduce costs and time in alloy development, enabling faster innovation in high-performance materials.

Mathematical models are also invaluable in simulating various manufacturing processes, including casting, forging, and welding, which are essential in shaping aluminum alloys into functional components. These simulations help optimize process parameters, such as temperature, cooling rates, and applied stresses, to achieve the desired microstructure and properties in the final product.

In casting, models of solidification and cooling are used to predict grain size, phase formation, and potential defects such as porosity or segregation. These models can be applied to optimize mold designs and cooling methods, ensuring uniformity and enhancing the mechanical properties of the cast alloy. Similarly, in forging, simulations can predict how the material will deform under different loads and temperatures, allowing for better control over the final microstructure and mechanical properties.

Welding processes, which are critical in joining aluminum alloys, benefit from models that simulate heat-affected zones, weld pool behavior, and residual stresses. By accurately predicting how the material will behave during welding, these models help minimize defects and optimize the strength of welded joints, crucial for structural integrity in high-stress applications.

Another significant area of application is additive manufacturing (AM) of aluminum alloys [10, 11], a rapidly growing field that allows for the production of complex geometries that are difficult to achieve with traditional methods. However, AM of aluminum alloys presents unique challenges, such as controlling solidification rates, minimizing defects like porosity, and ensuring the mechanical properties of the final product match those of conventionally processed materials. Mathematical models play a pivotal role in addressing these challenges by simulating the layer-by-layer build-up process, predicting temperature distribution, and

guiding the selection of process parameters to ensure optimal material properties. These models help in refining printing techniques and alloy compositions to improve the performance of 3D-printed aluminum parts used in aerospace, automotive, and other industries.

Several real-world applications highlight the effectiveness of mathematical models in alloy development and optimization.

One example is the development of high-strength aluminum alloys for aerospace applications. Through thermodynamic and mechanical property simulations, researchers have optimized aluminum-lithium (Al-Li) alloys for weight reduction and improved fuel efficiency in aircraft. By predicting the phase stability and microstructure evolution during processing, the models guided the selection of alloying elements, heat treatment parameters, and processing routes that resulted in alloys with enhanced strength-to-weight ratios while maintaining critical properties such as fatigue resistance and fracture toughness.

Another notable example is the development of automotive aluminum alloys. The automotive industry has a growing demand for lightweight materials to reduce vehicle weight and improve fuel efficiency. Mathematical models have been instrumental in developing aluminum alloys with high tensile strength and improved formability for use in structural components, such as body panels and chassis. Models have been used to predict the alloy's behavior under different manufacturing processes, such as stamping and extrusion, ensuring that the final product meets both performance and manufacturability requirements.

A third example is the optimization of aluminum alloys for additive manufacturing. The aerospace industry has increasingly adopted AM techniques for producing complex, lightweight components. Mathematical models have helped address challenges such as controlling the solidification process during 3D printing and minimizing the occurrence of defects such as cracks and porosity. By simulating the thermal and mechanical behavior of aluminum alloys during AM processes, models have enabled the development of new alloy compositions and optimized processing conditions, leading to the production of high-performance, near-net-shape components for critical applications.

These case studies demonstrate the potential of mathematical modeling to drive innovation in aluminum alloy design, manufacturing, and performance optimization across diverse industries. By integrating computational tools with experimental data, researchers and engineers can accelerate the development of advanced materials and optimize manufacturing processes, ensuring that aluminum alloys continue to meet the growing demands of modern applications.

5. Results and Discussion

Accuracy of Phase Prediction and Mechanical Property Simulations: The comparison between model predictions and experimental results demonstrates the effectiveness of mathematical modeling in understanding and designing aluminum alloys. Thermodynamic models, particularly CALPHAD-based approaches, accurately predict phase stability and equilibrium compositions in multi-component systems. For instance, the predicted phase diagrams for Al-Mg-Si and Al-Zn-Mg-Cu alloys align closely with experimental observations, enabling the identification of critical phase transformations during heat treatment.

Mechanical property simulations, such as stress-strain modeling and fatigue life prediction, also show high reliability. Stress-strain curves generated through finite element simulations closely match experimental tensile test results, confirming the models' ability to capture material deformation behavior under various loading conditions. Similarly, fatigue and creep models provide reasonable estimates of performance under cyclic and high-temperature conditions.

Limitations and Areas for Improvement: Despite their success, the models reveal certain limitations. Thermodynamic predictions occasionally diverge for systems involving rare alloying elements or under extreme processing conditions, highlighting gaps in existing

thermodynamic databases. Kinetic models face challenges in capturing complex multi-scale diffusion phenomena and rapid solidification during additive manufacturing. Moreover, mechanical property simulations require more robust constitutive equations to account for microstructural inhomogeneity and anisotropy. Future efforts should focus on expanding material databases, refining algorithms, and incorporating real-time experimental feedback to improve model accuracy.

Effect of Alloying Elements on Microstructure and Performance: The models provide valuable insights into the role of alloying elements in aluminum alloys. For example, magnesium in Al-Mg alloys enhances strength through solid-solution strengthening, while silicon in Al-Si alloys promotes wear resistance via the formation of hard, eutectic phases. Similarly, copper additions in Al-Cu alloys improve age-hardening potential, and lithium in Al-Li alloys reduces density and improves stiffness. These predictions align well with experimental microstructure analyses, showcasing the ability of models to guide composition optimization.

Observations on Process-Structure-Property Relationships: Mathematical modeling elucidates the intricate relationships between processing conditions, microstructure, and material properties. For example, simulations reveal how controlled cooling rates during casting influence grain size and dendritic arm spacing, which in turn affect strength and ductility. Kinetic models of precipitation hardening show how variations in heat treatment schedules impact precipitate size, distribution, and phase stability, ultimately dictating mechanical performance.

In additive manufacturing, models demonstrate the sensitivity of microstructure to thermal gradients and solidification rates, providing guidelines for optimizing process parameters to achieve uniform properties. These observations underscore the utility of mathematical models in predicting and tailoring the process-structure-property relationships essential for advanced alloy design and manufacturing.

By bridging theoretical predictions with experimental validation, this study highlights the strengths and limitations of current mathematical models for aluminum alloys. The results confirm their pivotal role in enabling data-driven alloy design, while also identifying areas for refinement to further enhance their predictive power.

6. Results Challenges and Future Directions and Discussion

Complexity of Multi-Component Systems: One of the significant challenges in modeling aluminum alloys lies in the complexity of multi-component systems. As the number of alloying elements increases, the interactions between them become highly intricate, making it difficult to accurately predict phase stability and microstructural evolution. Existing thermodynamic and kinetic models, while robust, often struggle to capture these interactions comprehensively, especially when unconventional or exotic elements are introduced into the system.

Data Scarcity for Less-Studied Alloying Elements: Another key limitation is the lack of high-quality data for less-studied alloying elements and their interactions with aluminum. Many emerging alloy systems, particularly those involving rare earth elements or novel additions, lack sufficient experimental data to populate thermodynamic databases or validate kinetic and mechanical models. This scarcity hampers the development and refinement of accurate predictive tools, slowing the exploration of new alloy designs.

Integration of AI and Machine Learning [12, 13] with Traditional Modeling: The integration of artificial intelligence (AI) and machine learning (ML) with traditional modeling techniques is an exciting trend that promises to address some of the aforementioned challenges. ML algorithms can process large datasets to uncover patterns and correlations that may not be evident through conventional methods. For example, neural networks can predict alloy properties based on limited experimental data,

augmenting traditional models like CALPHAD. Additionally, these tools can be used to optimize manufacturing processes, identify ideal compositions, and reduce computational costs.

Real-Time Simulation for Adaptive Manufacturing: Advancements in computational power and sensor technology are paving the way for real-time simulations that can be used in adaptive manufacturing. Such systems allow for dynamic adjustments to processing parameters based on live feedback, ensuring consistent quality and reducing defects. For example, real-time thermal simulations during additive manufacturing can help mitigate porosity and residual stresses. This adaptive approach requires highly accurate, fast, and integrated models, combining thermodynamics, kinetics, and mechanical simulations.

Exploration of Novel Alloys for Advanced Applications: Mathematical modeling opens new avenues for designing novel aluminum alloys tailored for advanced applications, such as aerospace, renewable energy, and electronics. For instance, high-temperature-resistant alloys for jet engines or conductive alloys for electric vehicle components could be developed more efficiently by leveraging predictive models. Exploring the use of rare earth elements, lightweight reinforcements, or unconventional compositions is a promising area where modeling can significantly accelerate progress.

Expansion of Models to Consider Environmental Factors: Future advancements should also focus on incorporating environmental factors into alloy models. For instance, models predicting corrosion resistance could be expanded to include the effects of varying environmental conditions, such as temperature, humidity, and exposure to aggressive chemicals. These capabilities would be invaluable for applications in marine environments, chemical processing, and sustainable construction. Furthermore, the incorporation of lifecycle analysis into alloy models could support the design of materials that balance performance with recyclability and environmental impact.

By addressing current challenges and capitalizing on emerging trends, mathematical modeling can continue to transform the field of aluminum alloy development. With ongoing advancements in computational methods, data integration, and experimental techniques, the future holds immense potential for the design and optimization of next-generation materials.

7. Conclusion

Mathematical modeling has emerged as a transformative tool in the advancement of aluminum alloy technology. By enabling precise predictions of phase stability, microstructural evolution, and mechanical behavior, these models significantly accelerate the design and optimization of alloys for diverse industrial applications. From lightweight aerospace components to high-strength automotive parts, modeling approaches such as thermodynamic simulations, kinetic analyses, and machine learning-driven predictions have reduced reliance on costly and time-consuming empirical methods. The integration of computational tools into alloy design pipelines has enhanced material performance while promoting efficiency and sustainability in manufacturing processes.

Despite these achievements, challenges remain in addressing the complexity of multi-component systems and improving model accuracy for unconventional alloying elements and extreme processing conditions. Data limitations, particularly for emerging alloys, highlight the need for more extensive experimental databases.

To fully realize the potential of mathematical modeling, future research should focus on refining existing techniques and expanding their scope. This includes integrating machine learning and artificial intelligence to complement traditional modeling methods, enabling the exploration of vast design spaces and the optimization of adaptive manufacturing processes. Additionally, incorporating environmental and sustainability factors, such as corrosion resistance and recyclability, into alloy models will ensure the relevance of these tools in addressing modern engineering challenges.

By addressing these areas, mathematical modeling will continue to drive innovation in aluminum alloy technology, fostering the development of next-generation materials that meet the demands of performance, sustainability, and efficiency in an increasingly competitive global market.

8. References

1. A. Bouzekova-Penkova, A. Miteva, Some aerospace applications of 7075 (B95) aluminium alloy, *Aerospace Research in Bulgaria*, **34**, 165-179 (2022).
2. W. Yi, J. Gao, L. Zhang, A CALPHAD thermodynamic model for multicomponent alloys under pressure and its application in pressurized solidified Al–Si–Mg alloys. *Advanced Powder Materials*, **3**(3), 100182 (2024).
3. W. Zhang, Y. Tang, J. Gao, et al., Determination of hardness and Young's modulus in fcc Cu–Ni–Sn–Al alloys via high-throughput experiments, CALPHAD approach and machine learning, *Journal of Materials Research and Technology*, **30**, 5381-5393, (2024).
4. R. Shi, A. A. Luo, Applications of CALPHAD modeling and databases in advanced lightweight metallic materials. *Calphad*, **62**, 1-17 (2018).
5. C. R. Hutchinson, Modeling the kinetics of precipitation in aluminium alloys, In *Fundamentals of Aluminium Metallurgy* (422-467, Woodhead Publishing, 2011).
6. Q. Du, L. Jia, K. Tang, B. Holmedal, Modelling and experimental validation of microstructure evolution during the cooling stage of homogenization heat treatment of Al–Mg–Si alloys. *Materialia*, **4**, 70-80 (2018).
7. Lan, Q., Wang, X., Sun, J., Chang, Z., Deng, Q., Sun, Q., Liu, Z., L. Yuan, J. Wang, Y. Wu, B. Liu, Artificial neural network approach for mechanical properties prediction of as-cast A380 aluminum alloy. *Materials Today Communications*, **31**, 103301 (2022).
8. E. S. Marques, F. J. Silva, A. B. Pereira, Comparison of finite element methods in fusion welding processes—A review, *Metals*, **10**(1), 75 (2020).
9. S. Geng, P. Jiang, L. Guo, et al., Multi-scale simulation of grain/sub-grain structure evolution during solidification in laser welding of aluminum alloys, *International Journal of Heat and Mass Transfer*, **149**, 119252 (2020).
10. M. M. Francois, A. Sun, W. E. King, et al., Modeling of additive manufacturing processes for metals: Challenges and opportunities, *Current Opinion in Solid State and Materials Science*, **21**(4), 198-206 (2017).
11. A. Hamrani, A. Agarwal, A. Allouhi, et al., Applying machine learning to wire arc additive manufacturing: a systematic data-driven literature review, *Journal of Intelligent Manufacturing*, **35**(6), 2407-2439 (2024).
12. M. Hu, Q. Tan, R. Knibbe, et al., Recent applications of machine learning in alloy design: A review, *Materials Science and Engineering: R: Reports*, **155**, 100746 (2023).
13. X. Liu, P. Xu, J. Zhao, et al., Material machine learning for alloys: Applications, challenges and perspectives, *Journal of Alloys and Compounds*, **921**, 165984 (2022).

Solution of the system of equations of energy and mass transfer with account of volumetric heat sources

Renat A. Sadykov¹, Airat L. Osipov¹, Artem V. Akhmerov¹

¹ Kazan State Power Engineering University, st. Krasnoselskaya, 51, 420066, Kazan, Russia
E-mail: sadykov_r_a@mail.ru, nord7077@yandex.ru, akhm@mail.ru

Abstract: The paper considers an analytical method for solving systems of equations of conjugate non-stationary heat and mass transfer with account of volumetric negative or positive heat sources (and steam generation as well). The obtained data can be used to find integral kinetic dependencies of heat and mass exchange processes, analytical formulas for calculating heat and mass transfer coefficients and other derivative quantities necessary for engineering calculations of processes and devices in chemical technology, biotechnology, industrial heat power engineering and other industries.

KEY WORDS: HEAT AND MASS TRANSFER, POTENTIAL, DIFFERENTIAL EQUATIONS, SYSTEM, MATRIX, SOLUTION, CALCULATION.

1. Introduction

The properties of the product at the outlet of the apparatus and the choice of the optimal technological mode of its processing are determined mainly by the interconnected irreversible processes occurring inside the contact (boundary) layer of the processed material (heat and mass transfer) and in the boundary layer of the environment (heating wall, air, inert coolant, steam, catalyst, etc.), since changes in the parameters of the environment change the conditions of substance transfer in the entire system, and the intensification or reduction of physicochemical and phase transformations in the material affects the structure of the boundary layer. Qualitative analysis of the mechanism of transfer processes is associated with finding non-stationary fields of transfer potentials (temperature, concentration, pressure, etc.), the evolution of which makes it possible to theoretically study the kinetics and dynamics of the process and outline the optimal conditions for its implementation.

Modern intensification of material processing technology leads to an increase in the role of non-stationary interconnected exchange processes compared to stationary and unrelated ones. This fact has not yet been sufficiently reflected in the field of solving energy and mass transfer (EMT) problems during short-term phase contact (SPC), when the Fourier criterion $Fo \leq 0.1$ [1,2].

2. Main Body

Interconnected energy and mass transfer in a stationary medium within the framework of linear nonequilibrium thermodynamics, in the general case, can be written through the vector of transfer potentials $\bar{\Pi}$ in the following one-dimensional dimensionless vector-matrix form:

$$\bar{\Pi}_{Fo} = [K] \bar{\Pi}_{xx} + \bar{I}(X, Fo), \quad (1)$$

or in scalar notation

$$\frac{\partial \Pi_i(X, Fo)}{\partial Fo} = \sum_{j=1}^n k_{ij} \frac{\partial \Pi_j(X, Fo)}{\partial X^2} + I_i(X, Fo) \quad i = \overline{1, n}, \quad (2)$$

where Π_i are the transfer potentials (system state parameters), $I_i(X, Fo)$ are the volumetric dimensionless powers of the sources (or sinks) of the i -th substance, caused by phase or other transformations, the elements of the matrix K are dimensionless quantities that are expressed through the similarity criteria of heat and mass transfer, X is the generalized coordinate, Fo is the generalized time.

To solve this system, we will use the method of constructing integrable combinations, which is used quite successfully to solve systems of ordinary differential equations (ODE) [2].

The use of such transformations in solving complex systems of equations describing the kinetics of irreversible processes allows one to use a wide class of known solutions of "pure" heat or mass conductivity to study various interrelated transport phenomena [2]. Let us consider the system of equations (3):

$$\begin{cases} \frac{\partial \Pi_1}{\partial Fo} = k_{11} \frac{\partial^2 \Pi_1}{\partial X^2} + k_{12} \frac{\partial^2 \Pi_2}{\partial X^2} + \dots + k_{1n} \frac{\partial^2 \Pi_n}{\partial X^2} + I_1 \\ \frac{\partial \Pi_2}{\partial Fo} = k_{21} \frac{\partial^2 \Pi_1}{\partial X^2} + k_{22} \frac{\partial^2 \Pi_2}{\partial X^2} + \dots + k_{2n} \frac{\partial^2 \Pi_n}{\partial X^2} + I_2 \\ \dots \\ \frac{\partial \Pi_n}{\partial Fo} = k_{n1} \frac{\partial^2 \Pi_1}{\partial X^2} + k_{n2} \frac{\partial^2 \Pi_2}{\partial X^2} + \dots + k_{nn} \frac{\partial^2 \Pi_n}{\partial X^2} + I_n \end{cases}$$

Expressing the values $\frac{\partial^2 \Pi_i}{\partial X^2}$, ($i = \overline{1, n}$) of the system of equations (3), using Cramer's rule

$$\frac{\partial^2 \Pi_i}{\partial X^2} = \frac{\begin{vmatrix} k_{11} & \dots & \frac{\partial \Pi_1}{\partial Fo} - I_1 & \dots & k_{1n} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ k_{1n} & \dots & \frac{\partial \Pi_n}{\partial Fo} - I_n & \dots & k_{nn} \end{vmatrix}}{\det K}$$

we move on to the system:

$$\begin{cases} \frac{\partial^2 \Pi_1}{\partial X^2} = \frac{1}{\Delta} \sum_{i=1}^n \left[A(B^1) \frac{\partial \Pi_i}{\partial Fo} + A(B^1) I_i \right] \\ \frac{\partial^2 \Pi_2}{\partial X^2} = \frac{1}{\Delta} \sum_{i=1}^n \left[A(B^2) \frac{\partial \Pi_i}{\partial Fo} + A(B^2) I_i \right] \\ \dots \\ \frac{\partial^2 \Pi_n}{\partial X^2} = \frac{1}{\Delta} \sum_{i=1}^n \left[A(B^n) \frac{\partial \Pi_i}{\partial Fo} + A(B^n) I_i \right] \end{cases}, \quad (4)$$

where B is the extended matrix for the matrix K has the following form

$$\begin{bmatrix} \frac{\partial \Pi_1}{\partial Fo} - I_1 & k_{11} & \dots & k_{1i+1} & \dots & k_{1n} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \frac{\partial \Pi_n}{\partial Fo} - I_n & k_{1n} & \dots & k_{ni+1} & \dots & k_{nn} \end{bmatrix}$$

$\Delta = \det K$, $A(B^j)$ ($j = \overline{1, n}$) are the algebraic complements of the corresponding elements of the matrices B^j .

Next, multiplying each of the equations of system (4) by some constant p_i ($i = \overline{1, n}$), and adding them together, we obtain:

$$\begin{aligned} \frac{\partial^2}{\partial X^2} (\sum_{i=1}^n p_i \Pi_i) = \\ \frac{1}{\Delta} \left(\frac{\partial}{\partial Fo} [\sum_{i=1}^n p_i \sum_{j=1}^n A(B^j) p_j] + \sum_{i=1}^n I_i \sum_{j=1}^n A(B^j) p_j \right) \end{aligned} \quad (5)$$

Equation (5) has the form of a heat conduction equation with respect to $Z = \sum_{i=1}^n p_i \Pi_i$, provided that

$$v^2 = \frac{(\sum_{j=1}^n A(B^j) p_j)_{n_j}}{\Delta p_j} \quad j = \overline{1, n}, \quad (6)$$

where the numbers v^2 and p_i are constants that are expressed through the elements of the matrix K included in the system of equations (1).

Excluding the relations of the type $\frac{p_i}{p_{i+1}}$ from equations (6), we obtain an equation of the j -th order for determining the eigenvalues of v_j^2 . Using the numbers $v_1^2, v_2^2, \dots, v_n^2$ successively found from this equation in equalities (6), we obtain $(n^2 - n)$ independent equations for calculating n^2 unknown numbers. Setting in them $p_{ii} = 1, (i = \overline{1, n})$, we obtain a square matrix

$$P = \begin{bmatrix} 1 & p_{12} & \cdot & \cdot & \cdot & p_{1n} \\ p_{21} & 1 & \cdot & \cdot & \cdot & p_{2n} \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ p_{n1} & \cdot & \cdot & \cdot & \cdot & 1 \end{bmatrix}, \quad (7)$$

from which we find the values of p_{ji}

Thus, the system of equations (1) can be rewritten as the following equivalent system of «unrelated» equations

$$\frac{\partial^2}{\partial X^2} Z_j = v_j^2 \frac{\partial}{\partial F_0} Z_j + v_j^2 M_j \quad (j = \overline{1, n}). \quad (8)$$

Setting $\frac{1}{v_j^2} = K_{jj}$, we finally obtain:

$$\begin{cases} \frac{\partial^2}{\partial X^2} Z_j = v_j^2 \left(\frac{\partial}{\partial F_0} Z_j - M_j \right) & (j = \overline{1, n}) \\ Z_j = \sum_{i=1}^n p_{ji} \Pi_i(X, F_0) \\ M_j = \sum_{i=1}^n p_{ji} I_i(X, F_0) \end{cases}, \quad (9)$$

Solving the equations of system (9) under the corresponding boundary conditions, we find solutions for the combined function Z_j . Denoting these solutions respectively through f_j , then the functions Π_j , are expressed directly through the functions f_j , as follows:

$$\Pi_j = \frac{\det P_j^f}{\det P}, \quad (10)$$

where P_j^f is the matrix P whose j -th column is replaced by the column of solutions f_j .

3. Conclusions

The proposed solution of problem (1) in the form (10) is of practical interest in calculating the rates of change of the corresponding transfer potentials. They allow one to quite simply link the problems of interrelated transfer with the problems of the classical theory of heat conduction and diffusion, determine the degree of influence of individual factors on the course of development of the process and, as a result, obtain simplified analytical expressions that are so necessary for engineering practice.

The results obtained serve the development of the general theory of mathematical modeling and can be useful in setting up experimental studies on non-stationary heat and mass transfer, in the analysis and calculation of exchange processes in industry and design [3-7].

4. References

- [1] Sadykov R.A. *Transfer processes during short-term phase contact*. Kazan, KGEU, 2004, -176 p.
- [2] Matveyev N.M. *Methods of integration of ordinary differential equations*. M., 1974, -564 p.
- [3] Lykov A.V., Mikhailov Yu.A. *Theory of heat and mass transfer*. M.-L.: Gosenergoizdat, 1963. 536 p.
- [4] Polyanin A.D., Zaitsev V.F. *Handbook of nonlinear equations of mathematical physics*. M.: FIZMATLIT, 2002, 432 p.
- [5] Tikhonov A.N., Samarskii A.A. *Equations of mathematical physics*. M.: Nauka, 1977, 736 p.
- [6] Migunov V.V., Sadykov R.A. *Characteristics of drying processes during short-term contact of wet material with a heating wall*.// TOHT, 1985, Vol.19, No. 1, 103-105.
- [7] Elsgolts L.I.E. *Differential equations and calculus of variations (series: "Course of higher mathematics and mathematical physics")* Moscow: Nauka, 1969, 424 p.

Educational Support by Grandparents and Human Capital Growth: An OLG Model with Endogenous Time Allocation

Mauro Maria Baldi^{1,*}, Raffaella Coppier¹, Elisabetta Michetti¹
University of Macerata, Macerata, Italy¹
mauromaria.baldi@unimc.it^{*}

Abstract: This study explores the role of grandparents in the education of their grandchildren within an overlapping generations model. We introduce an endogenously determined time allocation, where grandparents decide how much time to dedicate to their grandchildren's education based on a trade-off between leisure and educational contributions. The model shows that grandparental involvement in education influences the intergenerational transmission of human capital, with the potential for long-term effects on economic outcomes. By combining theoretical analysis and simulations, we highlight the dynamic relationship between grandparental education, human capital development, and the generational transmission process.

Keywords: OVERLAPPING GENERATIONS MODELS, ENDOGENOUS TIME ALLOCATION, EDUCATIONAL SUPPORT, FAMILY ECONOMICS, DYNAMICAL SYSTEMS

1. Introduction

The increasing longevity of the population has led to significant changes in family dynamics, especially regarding the role of grandparents in the education of their grandchildren. As life expectancy rises, grandparents are increasingly able to form extended relationships with their grandchildren, providing more opportunities to influence their educational outcomes. This paper explores the role of grandparents in the intergenerational transmission of human capital, focusing on the endogeneity of the time that grandparents dedicate to their grandchildren's education. Unlike in Baldi et al. [1], where this time was considered a fixed portion, in the present work we treat it as a variable determined by the trade-off between leisure and the desire to contribute to grandchildren's upbringing. In our overlapping generations model, we examine how the time grandparents invest in education, along with their own human capital, affects the educational outcomes of younger generations. Our findings suggest that grandparental involvement significantly shapes the human capital of grandchildren, influencing their cognitive development and academic achievements. This model provides new insights into how such intergenerational contributions might affect the transmission of education over time, ultimately impacting long-term social and economic outcomes [2, 3].

This article is structured as follows: in section 2, we introduce the model along with the tools used for its solution. Section 3 presents the solution of the model. Section 4 provides a discussion of the results, both from a theoretical and analytical perspective. Finally, we conclude in section 5.

2. Prerequisites and means for solving the problem

We analyze an Overlapping Generations (OLG) model where agents live for three periods: childhood, adulthood, and old age. In each period, agents make decisions related to consumption, time allocation, and child-rearing, with special attention to the role of grandparents in the education of grandchildren.

The economy at time t consists of three types of agents: the old (N_{t-1}), the adults (N_t), and the young (N_{t+1}), with the number of young agents evolving according to the number of children per adult, n_t , at time t . Specifically, the population evolves as:

$$N_{t+1} = n_t N_t. \quad (1)$$

Adults allocate their time between work and child-rearing, with a special focus on the educational role played by grandparents. In retirement, the elderly divide their time between leisure and educating grandchildren. This model highlights how this time allocation, particularly the time spent educating grandchildren, is influenced by the level of human capital, denoted by h_t , which is dependent on the educational investments of both parents and grandparents.

At time t , an adult maximizes utility from various factors: consumption during adulthood and old age, the number of children, the human capital of children, leisure time, and the time spent educating grandchildren. The adult's utility function U_t is given by:

$$\ln c_{1,t} + \rho \ln c_{2,t+1} + \theta \ln l_{t+1} + \frac{h_t}{h_{t-1}} \ln \mu_{t+1} + \beta \ln h_{t+1} + \lambda \ln n_t, \quad (2)$$

where:

- ❖ $c_{1,t} > 0$ represents consumption during adulthood,
- ❖ $c_{2,t+1} > 0$ represents consumption during old age,
- ❖ $n_t > 0$ is the number of children,
- ❖ $h_{t+1} > 0$ is the human capital of the offspring,
- ❖ $\mu_{t+1} \in (0, 1)$ represents the time fraction devoted to educating grandchildren during retirement,
- ❖ $l_{t+1} \in (0, 1)$ represents the time fraction devoted to leisure during retirement,
- ❖ $\rho \in (0, 1)$ represents the discount factor, reflecting the preference for future consumption over present consumption,
- ❖ $\lambda \in (0, 1)$ reflects the preference for the number of children, capturing the desire for larger family size,
- ❖ $\beta \in (0, 1)$ denotes the weight placed on child quality, as measured by the human capital of the next generation,
- ❖ $\theta > 0$ indicates the value placed on leisure time in old age.

Moreover, $\frac{h_t}{h_{t-1}}$ in (2) reflects human capital growth between generations.

The model also incorporates the cost of child-rearing and education into the budget constraints. Specifically, adults' available income at time t , determined by their wage rate $w_t > 0$ and human capital level $h_t > 0$, must cover various expenses. Here, w_t represents the wage rate per unit of labor at time t , so that the total income for an adult with human capital h_t is given by $w_t h_t$. This income must cover consumption in adulthood, $c_{1,t}$; savings $s_t \geq 0$; and the expenses associated with raising and educating children, which depend on the number of children $n_t > 0$. These costs include a fixed portion, $z \in (0, 1)$, of the adult's income dedicated to child-rearing, as well as an educational expenditure per child, $e_t \geq 0$. Thus, the budget constraint during adulthood is expressed as

$$c_{1,t} + s_t + n_t(e_t + zw_t h_t) = w_t h_t. \quad (3)$$

During retirement, old agents fund their consumption, $c_{2,t+1}$, using the returns from their previous savings. This relationship is captured by

$$c_{2,t+1} = r_{t+1}s_t, \quad (4)$$

where r_{t+1} is the interest factor at time $t+1$, and, again, s_t represents the accumulated savings from adulthood.

The education of children depends on three factors: parental investment in formal education, the time grandparents allocate to teaching grandchildren, and the overall human capital in society. Specifically, we assume that the contribution of grandparents and parents to the formation of children's human capital are perfect substitutes. In fact, the production function of human capital is given by:

$$h_{t+1} = \pi \left(h_{t-1} \frac{\mu_t}{n_t} + \phi e_t \right)^\delta \bar{h}_t^{1-\delta}, \quad (5)$$

where $\pi > 0$ and $\phi > 0$ are parameters influencing the effectiveness of grandparent time and educational investment, $\delta \in (0, 1)$ reflects the role of grandparents and parents in human capital accumulation, and $\bar{h}_t > 0$ represents the average human capital in society.

Finally, given the definitions of μ_{t+1} as the time fraction devoted to educating grandchildren and l_{t+1} as the time allocated to leisure, we must have:

$$\mu_{t+1} + l_{t+1} = 1. \quad (6)$$

To summarize, the overall model consists in maximizing the utility function (2) under the aforementioned constraints, i.e.: (3)-(6), plus a non-negativity constraint on e_t , namely:

$$\max U_t(c_{1,t}, c_{2,t+1}, \mu_{t+1}, l_{t+1}, e_t, n_t) = \ln c_{1,t} + \rho \ln c_{2,t+1} + \theta \ln l_{t+1} + \frac{h_t}{h_{t-1}} \ln \mu_{t+1} + \beta \ln h_{t+1} + \lambda \ln n_t \quad (7)$$

subject to:

$$c_{1,t} + s_t + n_t(e_t + zw_t h_t) = w_t h_t \quad (8)$$

$$c_{2,t+1} = r_{t+1}s_t \quad (9)$$

$$h_{t+1} = \pi \left(h_{t-1} \frac{\mu_t}{n_t} + \phi e_t \right)^\delta \bar{h}_t^{1-\delta} \quad (10)$$

$$\mu_{t+1} + l_{t+1} = 1 \quad (11)$$

$$e_t \geq 0. \quad (12)$$

We also assume the existence of numerous competitive producers using a production technology with constant returns to scale, where capital fully depreciates after one period. In the OLG framework, this means that the depreciation rate of capital is set to 1, since each period corresponds to a generation lasting about 20-30 years, making it realistic to assume complete depreciation after one period (as in [4]). Therefore, the capital stock in a given period equals the savings accumulated in the previous period.

At time t , production relies on physical capital K_t and labor L_t . The total output Q_t is determined by the following Cobb-Douglas production function:

$$Q_t = F(K_t, L_t) = AK_t^\alpha L_t^{1-\alpha}, \quad (13)$$

where $A > 0$ represents total factor productivity, and $\alpha \in (0, 1)$ is the capital's contribution to output. Firms maximize profits $Q_t - w_t L_t - r_t K_t$, leading to the following conditions for wages and capital returns:

$$w_t = A(1 - \alpha) \frac{K_t^\alpha}{L_t^{1-\alpha}} \quad (14)$$

$$r_t = A\alpha \frac{K_t^{\alpha-1}}{L_t^{1-\alpha}}. \quad (15)$$

Following Hirazawa and Yakita [4], labor is defined as $L_t = h_t N_t$, and introducing $k_t = \frac{K_t}{N_t}$, we derive the following expressions for wages and returns:

$$w_t = A(1 - \alpha) \frac{k_t^\alpha}{h_t^{1-\alpha}} \quad (16)$$

$$r_t = A\alpha \frac{k_t^{\alpha-1}}{h_t^{1-\alpha}}. \quad (17)$$

Thus, assuming $K_{t+1} = s_t N_t$ and $N_{t+1} = n_t N_t$, we obtain:

$$k_{t+1} = \frac{K_{t+1}}{N_{t+1}} = \frac{s_t}{n_t}. \quad (18)$$

This formula also appears in [4].

Finally, as assumed by Kitaura and Yakita [5], under the condition that all agents within a generation are identical, we have that $\bar{h}_t = h_t$.

3. Solution of the examined problem

The proposed model is a constrained optimization model, as we aim to maximize the utility function (7) subject to the equality constraints (8)-(11) and the inequality constraint (12). If s_t is derived from (9), l_{t+1} from (11), and these are substituted along with the expression for h_{t+1} , a new reformulation of the model is obtained with a single equality constraint and one inequality constraint. This reformulation can be solved using the method of Lagrange multipliers: by associating a Lagrange multiplier with each constraint, the Lagrangian function associated with the new model can be constructed. It is easy to verify that for this model, the conditions of the Lagrange multiplier theorem are satisfied. Therefore, by setting the gradient of the Lagrangian function with respect to the decision variables $c_{1,t}$, $c_{2,t+1}$, μ_{t+1} , e_t , and n_t equal to zero and accounting for both the equality constraint and the complementary slackness conditions due to the inequality constraint, two systems are obtained, each of which holds in two regions of the set of solutions. This approach provides the so-called first-order conditions. These are necessary conditions within which to search for a local maximum. To also obtain sufficient conditions, it is necessary to impose that the Hessian matrix of the Lagrangian function is negative definite on the constraint set of the active constraints. Taking all these considerations into account, we obtain the aforementioned two regions, which are characterized, in addition to the inequality $\lambda - \beta\delta > 0$, by the following constraints:

$$\text{Region A: } \frac{w_t h_t}{\mu_t h_{t-1}} > \frac{1+\rho+\lambda-\beta\delta}{\beta\delta\phi}$$

$$\text{Region B: } \frac{w_t h_t}{\mu_t h_{t-1}} \leq \frac{1+\rho+\lambda-\beta\delta}{\beta\delta\phi}.$$

In region A, it holds that:

$$c_{1,t} = \frac{1}{1+\rho+\lambda-\beta\delta} \cdot \frac{h_{t-1}\mu_t + \phi w_t h_t}{\phi} \quad (19)$$

$$c_{2,t+1} = \frac{\rho}{1+\rho+\lambda-\beta\delta} \cdot \frac{h_{t-1}\mu_t + \phi w_t h_t}{\phi} r_{t+1} \quad (20)$$

$$s_t = \frac{\rho}{1+\rho+\lambda} \cdot \frac{h_{t-1}\mu_t + \phi w_t h_t}{\phi} \quad (21)$$

$$e_t = zw_t h_t \left(\frac{\beta\delta}{\lambda-\beta\delta} - \frac{1+\rho+\lambda}{\lambda-\beta\delta} \cdot \frac{h_{t-1}\mu_t}{h_{t-1}\mu_t + \phi w_t h_t} \right) \quad (22)$$

$$n_t = \frac{\lambda-\beta\delta}{1+\rho+\lambda} \cdot \frac{1}{zw_t h_t} \cdot \frac{h_{t-1}\mu_t + \phi w_t h_t}{\phi}, \quad (23)$$

while in region B, it holds that:

$$c_{1,t} = \frac{1}{1+\rho+\lambda-\beta\delta} w_t h_t \quad (24)$$

$$c_{2,t+1} = \frac{\rho}{1+\rho+\lambda-\beta\delta} w_t h_t r_{t+1} \quad (25)$$

$$s_t = \frac{\rho}{1+\rho+\lambda-\beta\delta} w_t h_t \quad (26)$$

$$e_t = 0 \quad (27)$$

$$n_t = \frac{\lambda - \beta\delta}{1 + \rho + \lambda - \beta\delta} \cdot \frac{1}{z}. \quad (28)$$

Furthermore, in both regions it holds that:

$$\mu_{t+1} = \frac{h_t}{h_t + \theta h_{t-1}}. \quad (29)$$

4. Results and discussion

We focus only on region A for the remainder of this work, leaving region B for future study.

If we substitute the values of s_t and n_t from the first-order conditions into (18), we obtain the following equation:

$$k_{t+1} = \frac{\rho}{\lambda - \beta\delta} z w_t h_t. \quad (30)$$

Taking (30), (29) and (10) into account, and after appropriate substitutions, including (16), we obtain the following 3D discrete-time dynamic system:

$$T_A: \begin{cases} k_{t+1} = \frac{\rho}{\lambda - \beta\delta} z A(1 - \alpha) k_t^\alpha h_t^{1-\alpha} \end{cases} \quad (31)$$

$$\begin{cases} \mu_{t+1} = \frac{h_t}{h_t + \theta h_{t-1}} \end{cases} \quad (32)$$

$$\begin{cases} h_{t+1} = \pi \left[\frac{\beta\delta}{\lambda - \beta\delta} \phi z A(1 - \alpha) k_t^\alpha h_t^{1-\alpha} \right]^\delta h_t^{1-\delta}, \end{cases} \quad (33)$$

Where we have also exploited the assumption $\bar{h}_t = h_t$.

As in the works [1,6,7], it is useful to introduce the following variables: $x_t = \frac{k_t}{h_t}$ and $y_t = \frac{h_t}{h_{t-1}}$, which respectively represent the physical capital/human capital ratio and the human capital growth rate.

With the second-order condition $\lambda - \beta\delta > 0$ in mind, and using these substitutions, we can redefine region A as follows:

$$A(1 - \alpha) \frac{x_t^\alpha y_t}{\mu_t} > \frac{1 + \rho + \lambda - \beta\delta}{\beta\delta\phi}. \quad (34)$$

Additionally, we can reformulate the system T_A as follows:

$$S_A: \begin{cases} x_{t+1} = \frac{\rho}{\pi\beta\delta\phi} \left[\frac{\beta\delta\phi}{\lambda - \beta\delta} z A(1 - \alpha) x_t^\alpha \right]^{1-\delta} \end{cases} \quad (35)$$

$$\begin{cases} \mu_{t+1} = \frac{y_t}{y_t + \theta} \end{cases} \quad (36)$$

$$\begin{cases} y_{t+1} = \pi \left[\frac{\beta\delta\phi}{\lambda - \beta\delta} z A(1 - \alpha) x_t^\alpha \right]^\delta. \end{cases} \quad (37)$$

We observe that the nature of the system S_A is completely determined by equation (35). In fact, (37) is given by a constant multiplied by $x_t^{\alpha\delta}$, so if x_t converges, then y_t also converges. Conversely, if x_t diverges, then y_t also diverges. Furthermore, for (36), if y_t diverges, then μ_t converges to 1. Conversely, if y_t converges, then μ_t also converges. In both cases, μ_t converges. Based on the considerations just made, it is therefore sufficient to study the difference equation (35). In Proposition 1, we present the equilibrium points of (35) along with their stability.

Proposition 1. *The difference equation (35) has two equilibrium points: the origin, which is unstable, and the point*

$$x^* = \left\{ \frac{\rho}{\pi\beta\delta\phi} \left[\frac{\beta\delta\phi}{\lambda - \beta\delta} z A(1 - \alpha) \right]^{1-\delta} \right\}^{\frac{1}{1-\alpha(1-\delta)}}, \quad (38)$$

which is asymptotically stable.

Proof. Let $f(x_t) := \frac{\rho}{\pi\beta\delta\phi} \left[\frac{\beta\delta\phi}{\lambda - \beta\delta} z A(1 - \alpha) x_t^\alpha \right]^{1-\delta}$. Then, the equation $x = f(x)$ is clearly satisfied by $x = 0$, so the origin is an equilibrium point of the difference equation (35). Now, assuming $x \neq 0$, by dividing both sides of the equation $x = f(x)$ by x , we obtain

$$x^{1-\alpha(1-\delta)} = \frac{\rho}{\pi\beta\delta\phi} \left[\frac{\beta\delta\phi}{\lambda - \beta\delta} z A(1 - \alpha) \right]^{1-\delta}. \quad (39)$$

Raising both sides of (39) to the power of $\frac{1}{1-\alpha(1-\delta)}$, we obtain (38). As for the stability of the equilibrium points found, we need to know the first derivative (with respect to x_t) of the function f . It is given by:

$$f'(x_t) = \frac{\rho}{\pi\beta\delta\phi} \left[\frac{\beta\delta\phi}{\lambda - \beta\delta} z A(1 - \alpha) \right]^{1-\delta} \alpha(1 - \delta) x_t^{\alpha(1-\delta)-1}. \quad (40)$$

Since α and δ are between 0 and 1, the exponent of x_t in (40) is negative, and thus the first derivative of f is not defined for $x_t = 0$. For the same reason, it is clear that $\lim_{x_t \rightarrow 0^+} f'(x_t) = +\infty$ and thus the origin is an unstable equilibrium point. As for the equilibrium point x^* , it is easy to verify that $f'(x^*) = \alpha(1 - \delta)$. Since α and δ are between 0 and 1, their product is also between 0 and 1, and thus x^* is an asymptotically stable equilibrium point. ■

We would like to make an important observation following the results just proven. In fact, what was proven in Proposition 1 does not take into account region A, which in the new variables x_t and y_t is described by (34). We observe that if $x_t = 0$, then from (37) we also have $y_t = 0$, and thus (34) cannot be satisfied. Therefore, we can exclude the origin as an equilibrium point in region A. At this point, it is legitimate to ask whether the equilibrium point x^* also exists in region A. Proposition 2 provides an answer to this question.

Proposition 2. *There exists a combination of parameters such that the equilibrium point x^* belongs to region A.*

Proof. From (35)-(38), we have that the coordinates of the three-dimensional equilibrium point of the system S_A are given by x^* , by $y^* = \pi \left[\frac{\beta\delta\phi}{\lambda - \beta\delta} z A(1 - \alpha) \right]^\delta (x^*)^{\alpha\delta}$ and by $\mu^* = \frac{y^*}{y^* + \theta}$. Therefore, the inequality (34) evaluated at x^* , y^* , and μ^* can be rewritten as

$$A(1 - \alpha)(x^*)^\alpha (y^* + \theta) > \frac{1 + \rho + \lambda - \beta\delta}{\beta\delta\phi}. \quad (41)$$

Since x^* and y^* increase as A increases, it is evident that, given the parameters on the right-hand side of (41), there exists a sufficiently large value of A that satisfies (41). ■

To confirm what has been proven, we want to provide a numerical example starting from the following combination of parameters: $\alpha = 0.5$, $A = 10$, $\beta = 0.9$, $\delta = 0.9$, $\lambda = 0.9$, $z = 0.9$, $\phi = 0.5$, $\pi = 0.2$, $\rho = 0.2$, and $\theta = 0.8$. Let's begin by verifying that the equilibrium point inside region A exists. In fact, approximating to four decimal places, we find: $x^* = 3.5541$, $y^* = 5.3044$, and $\mu^* = 0.8689$. Substituting these values into (41), this inequality is satisfied.

With this parameter configuration, the map associated with (35) is shown in Fig. 1.

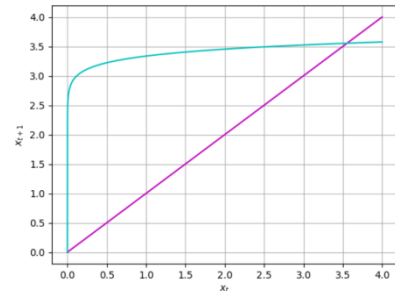


Fig. 1 The map of the difference equation (35) with the proposed parameter configuration.

As we mentioned, the origin is not part of region A, but if we only consider the difference equation (35), Fig. 1 provides clear graphical evidence that the origin is an unstable equilibrium point, since, as already proven in Proposition 1, the slope of the tangent line to the map at the origin tends to $+\infty$.

From Fig. 1, we can clearly observe that the slope of the tangent line at the interior fixed point is between 0 and 1, and thus this fixed point is asymptotically stable. Based on the reasoning in Proposition 1, and on the fact that the origin does not belong to region A, this fixed point is also globally asymptotically stable in region A.

In Fig. 2-4, we respectively show the evolution of x_t , μ_t , and y_t respectively, with the aforementioned parameter configuration, choosing $x_0 = 4$, $\mu_0 = 0.5$, and $y_0 = 6$. As clearly seen in Fig. 2 and in line with what was proven in Proposition 1, the orbit converges to the point $x^* = 3.5541$ after a few iterations. Furthermore, from Figure 3 it is evident that μ_t converges to $\mu^* = 0.8689$. Therefore, there is an equilibrium level of time allocation to which μ_t converges. Finally, from Figure 4 it can be observed that y_t converges to $y^* = 5.3044$.

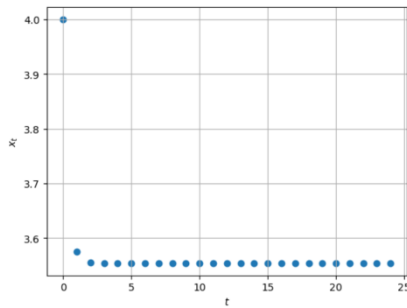


Fig. 2 The evolution of x_t with the proposed parameter configuration and the initial points **considered**.

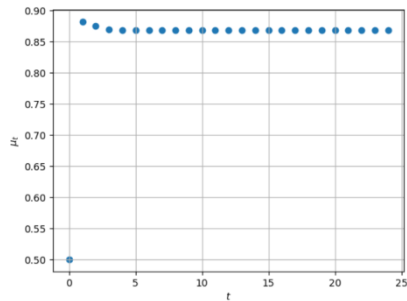


Fig. 3 The evolution of μ_t with the proposed parameter configuration and the initial points **considered**.

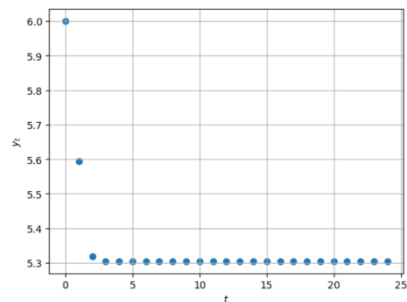


Fig. 4 The evolution of y_t with the proposed parameter configuration and the initial points **considered**.

5. Conclusion

This study highlights the growing significance of grandparents in the educational development of their grandchildren, driven by the increasing longevity of the population. As life expectancy rises, grandparents are more likely to form lasting relationships with their grandchildren, creating additional opportunities to influence their educational outcomes. This work is a natural evolution of Baldi et al. [1], where the time grandparents dedicate to their grandchildren's education was treated as a fixed parameter. In contrast, we consider this time as a variable, determined by the trade-off between leisure and the desire to contribute to their grandchildren's upbringing.

The model we developed provides new insights into how such contributions can affect the transmission of education over time, offering important implications for long-term social and economic outcomes.

Encouraged by the promising results, we plan to continue with this line of research. Possible developments include a different evolution of h_{t+1} or a scenario where grandparents dedicate their time to work with reduced productivity.

Acknowledgement

This work has been funded by the European Union - NextGenerationEU under the Italian Ministry of University and Research (MUR) National Innovation Ecosystem grant ECS00000041 - VITALITY - CUP D83C22000710005.

6. References

1. M. M. Baldi, R. Coppi, E. Michetti, Mathematical Social Sciences, 131, 67-79 (2024)
2. G. S. Becker, N. Tomes, Human capital and the rise and fall of families, 4 (3, part 2), S1-S39 (1986)
3. T. Bol, M. Kalmijn, Grandparents' resources and grandchildren's schooling: Does grandparental involvement moderate the grandparent effect?, Social Science Research, 55, 155-170 (2016)
4. M. Hirazawa, A. Yakita, Labor supply of elderly people, fertility, and economic development, Journal of Macroeconomics, 51, 75-96 (2017)
5. K. Kitaura, A. Yakita, Labor supply of elderly people, fertility, and economic development, Journal of Macroeconomics, 51, 75-96 (2017)
6. A. Yakita, Human capital accumulation, fertility and economic development, Journal of Economics, 99, 97-116 (2010)
7. K. Kitaura, A. Yakita, School education, learning-by-doing, and fertility in economic development, Review of Development Economics, 14, 736-749 (2010)

Applicability of cable theory to study of action potential propagation in cardiac tissue

Natela Zirakashvili

I. Vekua Institute of Applied Mathematics of Iv. Javakishvili Tbilisi State University, Georgia
natzira@yahoo.com

Abstract: Action potential propagation in cardiac tissue by using cable equations is studied. The work discusses a one-dimensional model of continuously coupled myocytes. Electrical behavior in cardiac tissue is averaged over many cells. Therefore, the transmembrane potential behavior for a single cell is studied. Using the monodomain model, in the absence of current at the beginning and end of the cable (cell), the initial-boundary problem is posed and solved analytically. The problem is solved by the method of separation of variables. Numerical modeling of transmembrane potential propagation is implemented. Transmembrane isopotential contours and graphs corresponding to the obtained numerical results are presented.

Keywords: CARDIOMYOCYTE, TRANSMEMBRANE POTENTIALS, PASSIVE 1D CABLE EQUATION, MONODOMAIN MODEL.

1. Introduction

Heart diseases are one of the leading causes of death in the world, and there are many scientific papers devoted to the study of the causes and mechanisms of heart problems. The article studies the propagation of action potential in cardiac tissue using the cable equation. Cable theory, one of the main problems of which is the calculation of the membrane potential and which has been developed in recent decades, is older than the cable equation itself. It is a variation of the equations developed by Lord Kelvin to model the propagation of electrical signals in underwater telegraphs. The cable theory was originally applied to conducting potentials in the axon, for example, by Hodgkin and Rushton [1]. Cardiomyocytes (heart muscle cells) differ from nerve axons in their shape and size - roughly they are very small cylinders.

The current work discusses a one-dimensional model of continuously coupled myocytes. In this case, the electrical behavior in cardiac tissue is averaged for many cells. So, the distribution of the transmembrane potential in a single cell is studied. Using a monodomain model, the propagation of the transmembrane potential in a thin cylindrical excitable myocyte is studied in the absence of current at the beginning and end of the myocyte. This problem is solved by the method of separation of variables. Numerical results of transmembrane potential propagation in cardiomyocytes are obtained using MATLAB software, and transmembrane isopotential contours and graphs of the obtained numerical results are presented.

2. Theoretical aspects

2.1. Problem formulation and principal formulas

The heart consists of transversely striated muscle tissue, which ensures the rapid spread of the wave of fiber contraction. As a result, all sections of the heart contract as a single entity. The homogeneous representation of cardiac tissue involves a large number of identical myocytes, which can be thought of as two interconnected spaces - intracellular and extracellular. The cells are connected by gap junctions (Fig. 1).

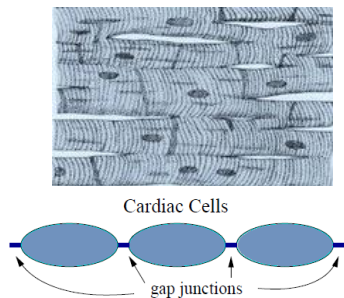


Fig. 1. Schematic drawing of cardiac tissue.

The cardiac muscle action potential (membrane potential) is a brief change in voltage on the cell membrane in heart cells caused by the movement of charged atoms (ions) into and out of the cell via proteins called ion channels. The cell membrane separates extracellular and intracellular spaces with potentials φ_e and φ_i , while $V = \varphi_i - \varphi_e$ is the transmembrane potential.

An action potential is an excitation wave, which as a brief change of the membrane potential in the membrane of a living cell moves to a small area of an excited cell (neuron or cardiomyocyte), as a result of which the outer surface of this area becomes negatively charged compared to the inner surface of the membrane, while it is positively charged in a non-excitation state. Sometimes the action potential is called a propagating potential because the excitation wave is actively transmitted along the fiber of a neuron or muscle cell. Cardiomyocytes are approximately cylindrical (very small, measured in microns) whose length (e.g., x in the direction of the cylinder's long axis) is sufficiently greater than its diameter. So we can assume that the action potential of the cell depends only on the length variable, and the problem can be reduced to a single measurement. Thus, the article discusses continuously coupled 1D myocyte models. Intracellular, extracellular, and transmembrane potentials are vector fields in space and time, i.e. $\varphi_i = \varphi_i(x, t)$, $\varphi_e = \varphi_e(x, t)$, $V = V(x, t)$.

The electrical behavior of the cell membrane of cardiac tissue and the propagation of the action potential is described by monodomain model (equations). Monodomain model use the representation of cardiac muscle as two interconnected spaces, intracellular φ_i and extracellular φ_e . The monodomain model ignores extracellular space and $V = \varphi_i$.

The passive cable equation will be written down as follows [2]:

$$\tau_m \frac{\partial V}{\partial t} = \lambda^2 \frac{\partial^2 V}{\partial x^2} - V, \quad (1)$$

where λ is the constant of the space (length) of the passive cable equation and is expressed by the following formula:

$$\lambda = \sqrt{r_m \sigma_i} = \sqrt{\frac{r_m}{r_i}}, \quad \tau \text{ is a time constant and is defined by the}$$

following formula: $\tau = r_m c_m$, r_i is specific resistance of the cell, r_m is membrane resistance and c_m is membrane capacity.

2.2. Problem statement and solution

Consider a thin cylindrical excitable cell of length L . Let us solve the passive cable equation (1) with the following boundary and initial conditions:

$$\text{For } x = 0: V_{,x}(x, t) = 0, \quad (2)$$

$$\text{For } x = L: V_{,x}(x, t) = 0,$$

$$\text{For } t = 0: V(x, 0) = f(x). \quad (3)$$

Using the method of separation of variables and considering the boundary (2) and initial (3) conditions, we will obtain the following expression [2]:

$$\begin{aligned}
 V(x, t) &= \frac{2}{L} \frac{L^2}{2} + \frac{2}{L} \sum_{n=1}^{\infty} \left[\frac{L^2}{\pi n} \sin(\pi n) + \left(\frac{L}{\pi n} \right)^2 (\cos \pi n - 1) \right] \cos\left(\frac{\pi n x}{L}\right) e^{\left(1 - (\lambda \pi n / L)^2\right) t / \tau_n} \\
 &= L + 2L \sum_{n=1}^{\infty} \left(\frac{1}{\pi n} \sin(\pi n) + \frac{1}{(\pi n)^2} (\cos \pi n - 1) \right) \cos\left(\frac{\pi n x}{L}\right) e^{\left(1 - (\lambda \pi n / L)^2\right) t / \tau_n}.
 \end{aligned}$$

3. Numerical simulation

The numerical simulation for the 1D model of continuously coupled myocytes in the absence of current at the beginning and end of the cable (cell), were performed using MATLAB software for the following data: time (τ ranges from 2.5 to 4.5 ms in humans) and length (λ ranges from 1.3 to 2.2 mm) for four pairs of constants: 1) $\tau = 2.5\text{ms}$, $\lambda = 1.3\text{mm}$; 2) $\tau = 2.8\text{ms}$, $\lambda = 1.6\text{mm}$; 3) $\tau = 3\text{ms}$, $\lambda = 1.8\text{mm}$ and 4) $\tau = 4.5\text{ms}$, $\lambda = 2.2\text{mm}$, myocyte (cell) length: $L = 135\mu\text{m} = 0.135\text{mm}$, spatial (lengthy) discretization of $\Delta x = 6\mu\text{m} = 0.006\text{mm}$ and temporal discretization of $\Delta t = 0.02\text{ms}$ was used. Numerical values of the transmembrane potential V were obtained during the variation of x (from 0.006mm to 0.135mm) and t (from 0.02ms to 0.03ms).

Fig. 2 shows myocyte transmembrane isopotential contours for four values of τ and λ . As Fig. 2 shows, the transmembrane isopotential contours in all four cases look similar, in particular, all of them are almost elliptic lines, and only their numerical values differ slightly.

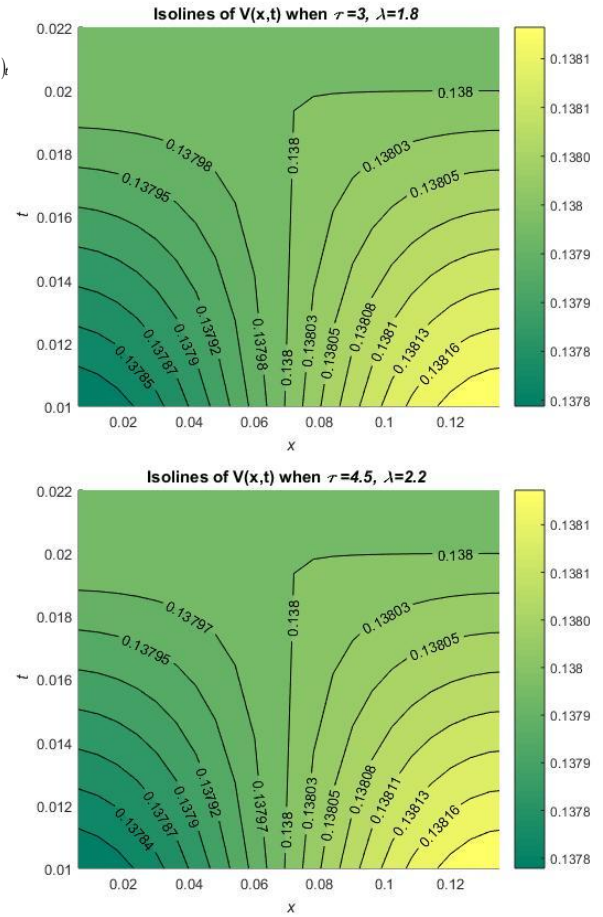


Fig. 2 Transmembrane isopotential contours for different fixed values of time and space constants.

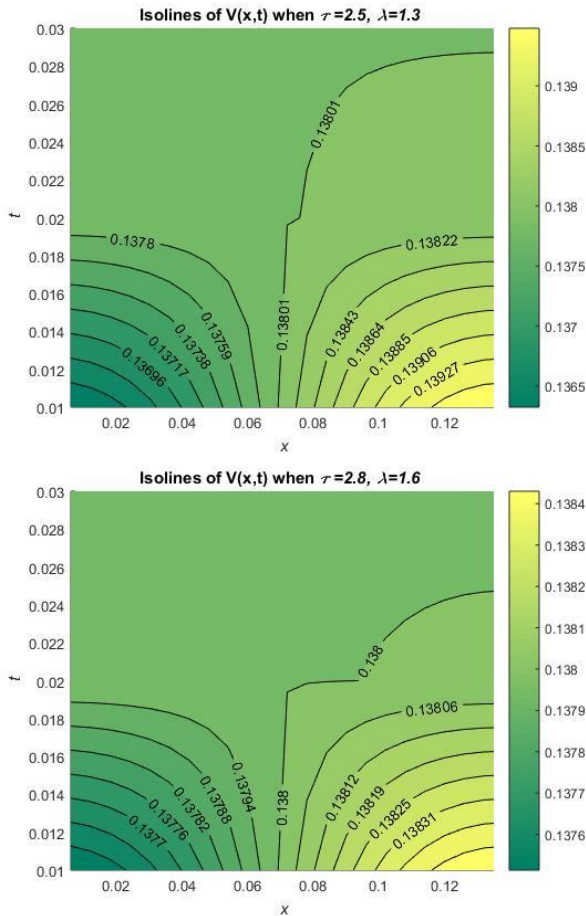
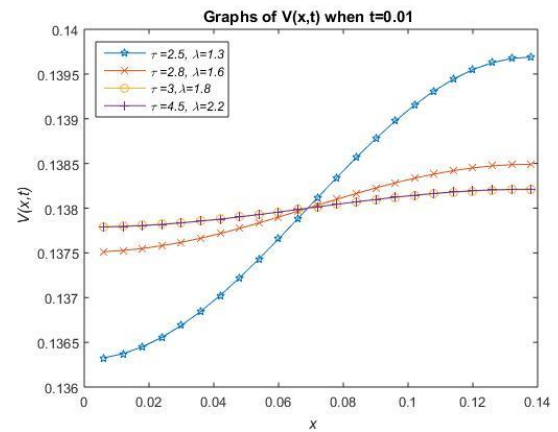


Fig. 3 gives the graphs of variation of V transmembrane potential along x for four different fixed constant values of τ and length λ and different fixed values of t , in particular: upper left figure: $t = 0.01\text{ms}$, upper right figure: $t = 0.02\text{ms}$, lower left figure: $t = 0.05\text{ms}$, lower right figure: $t = 0.09\text{ms}$. Fig. 4 shows: 1) as the value of t increases different fixed constant values of τ and length λ , the graph of variation of transmembrane potentials get close to each other meaning that the transmembrane potential will change after some time only slightly when τ and λ change; 2) in all four cases, as $x \approx 0.075$, for all four values of time and length constants, the transmembrane potential $V(x, t) = 0.138$.



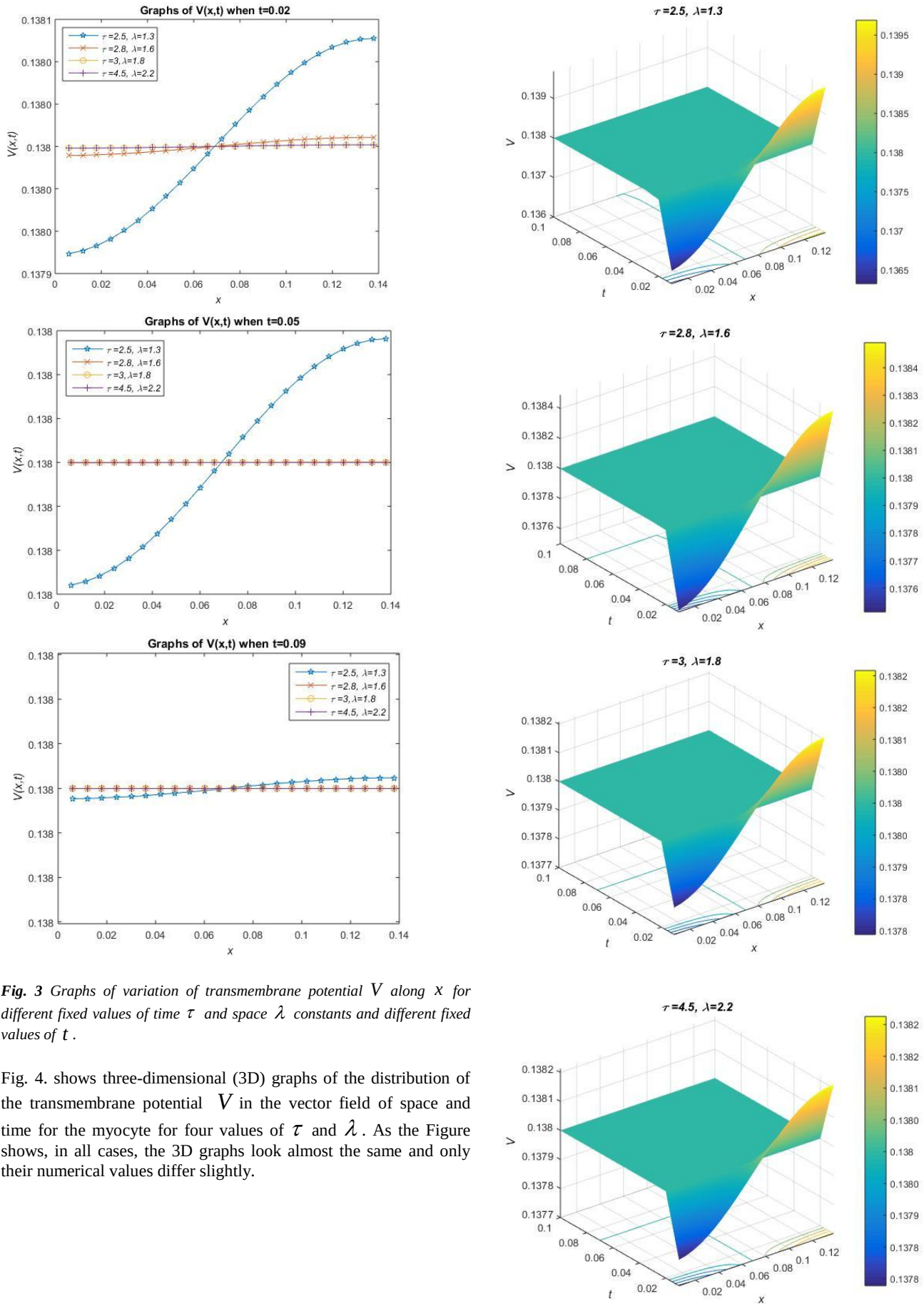


Fig. 3 Graphs of variation of transmembrane potential V along x for different fixed values of time τ and space λ constants and different fixed values of t .

Fig. 4. shows three-dimensional (3D) graphs of the distribution of the transmembrane potential V in the vector field of space and time for the myocyte for four values of τ and λ . As the Figure shows, in all cases, the 3D graphs look almost the same and only their numerical values differ slightly.

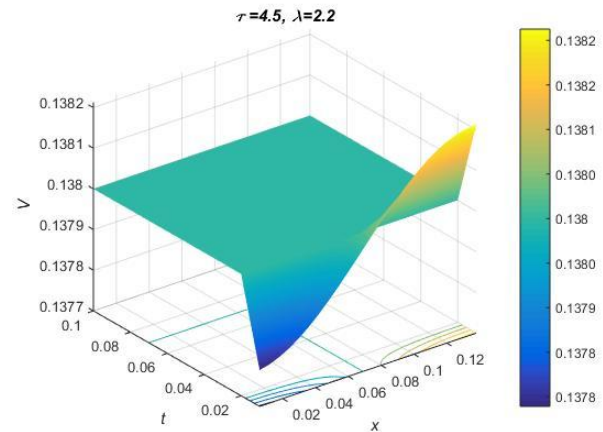


Fig.4. 3D graphs of distribution of V transmembrane potential in the x, t vector field for different fixed values of time and space constants

4. Conclusion

The transmembrane potential propagation for a single cell is studied; in particular, the transmembrane *potential* propagation of a thin cylindrical excitable cardiomyocyte in the absence of current at the beginning and end of the cardiomyocyte is studied. Using MATLAB software for the above problem, numerical results for the transmembrane potential are obtained, from which the contours of the transmembrane isopotential for the plane area in the vector field of length X and time t are construed. Some 2D and 3D graphs are plotted.

Cardiovascular disease remains the leading cause of death worldwide, most notably, heart failure due to heart attack and fatal arrhythmias. The immediate cause of fatal cardiac arrhythmias is still not thoroughly understood, but in many cases, it may be related to an improper spread of the cardiac action potential. It should be noted that, despite many years of research, the distribution of the action potential of the heart muscle is still not fully understood. So its study remains a pressing topic of many modern scientific studies.

5. References

1. Hodgkin, A.L., Rushton, W.A.H. The electrical constants of a crustacean nerve fiber. Proc Roy Soc B, **133**(873), 1946, 444-479.
2. Zirakashvili, N., Zirakashvili, T. Study of Action Potential Propagation in Cardiac Tissues Using Cable Theory. WSEAS TRANSACTIONS on BIOLOGY and BIOMEDICINE; **20**, 2023, 228-239.

Bayesian vs. frequentist inference – an ophthalmic study on ocular perfusion pressure

Biljana Tojtovska^{1,*}, Panche Ribarski¹, Antonela Ljubic², Galina Dimitrova³,

Faculty of Computer Science and Engineering, University Ss Cyril and Methodius Skopje, Republic of North Macedonia¹,

Department of Ophthalmology, Medika Plus Polyclinic, Skopje, Republic of North Macedonia²,

Department of Ophthalmology, City General Hospital “8th of September”, Skopje, Republic of North Macedonia³,

biljana.tojtovska@finki.ukim.mk*

Abstract: This study investigates the application of Bayesian statistical methods for comparing ocular perfusion pressure (OPP) between glaucoma and non-glaucoma populations, contrasting it with traditional frequentist approaches. Using OPP measurements from two patient groups, we employ partially informed Bayesian models to test the hypothesis of no difference in means between the groups. We calculate Bayes factor using Savage-Dickey density ratio and offer insights in the hypothesis beyond p-values. The results highlight the advantages of the Bayesian approach, including its flexibility in incorporating prior information and interpreting evidence. We discuss the limitations and potential biases introduced by the choice of priors. This paper contributes to the understanding of Bayesian inference in ophthalmic research and emphasizes its potential for hypothesis testing in clinical studies.

Keywords: OCULAR PERFUSION PRESSURE, BAYESIAN INFERENCE, FREQUENTIST STATISTICS, BAYES FACTOR, R, JAGS

1. Introduction

Classical statistical approach does not provide probabilistic quantification of the results of frequentist statistical methods. The interpretation of confidence intervals, p-values and null hypothesis testing is counterintuitive and often misunderstood from many researchers, especially in medical sciences. As a result, there are many misleading interpretations, especially when working with small sample sizes, multiple hypothesis testing or studies with limited power [1-4].

Bayesian inference addresses some of these key shortcomings of frequentist approach, by combining prior beliefs and observed data to generate posterior distributions of parameters. This is particularly valuable in medical research, where prior studies or expert opinions can inform the analysis. Bayesian methods allow for a direct probabilistic interpretation of parameters and results and even more, they give probabilistic quantification of uncertainty in predictions. Instead of relying on point estimates and confusing confidence intervals, the results from Bayesian analysis are given through a distribution of possible outcomes, credible intervals and Bayes factors. Bayesian inference allows the analysis to be updated with additional data, making it more adaptive and responsive to new information. This is especially important in medical research, where decisions and treatment should be updated as new scientific knowledge is available [5-7].

The goal of this study is to compare frequentist and Bayesian approaches in the analysis of data from an ophthalmic study. We analyze ocular perfusion pressure (OPP) in glaucoma and non-glaucoma patients, with a primary goal to assess whether there is a significant difference in the means of both populations. We present results from the frequentist statistical tests, discuss limitations and introduce the Bayesian approach based on Bayes factor. We consider three different models with prior parameter distributions, incorporating prior knowledge from previous studies. By comparing the results and interpretations of these approaches, we aim to highlight the strengths and limitations of each approach. This will also provide better understanding of Bayesian inference for medical studies.

The paper is organized as follows: In Chapter 2 we describe the data set and the variable of interest – ocular perfusion pressure. Chapter 3 discusses results from frequentists statistics, Chapter 4 introduces Bayes factor analyses where three models are described, and details of Bayes factor are given. Chapter 5 includes discussion and interpretation of the results as well as suggestions for future work. The conclusions of our study are presented in Chapter 6.

2. Data on ocular perfusion pressure in patients with and without primary open angle glaucoma

The data in this study is part of a greater dataset from our previous research on pressure related ocular parameters in patients with and without primary open angle glaucoma (POAG) [8]. This study included 27 patients with POAG and 30 patients in the control group without POAG. The goal of this broader study was to investigate differences in pressure related ocular parameters as intraocular pressure (IOP), OPP, and Translaminar Pressure Difference (TLDP) in both populations. The dataset consisted of 42 variables including age, sex, education data as well as different ophthalmic and systemic measurements.

In the current study we discuss only the data on OPP from both populations. OPP is an important hemodynamic parameter that is critical indicator of ocular blood flow. It is used to assess the risk of various eye conditions involving the optic nerve and retinal health. OPP can reflect underlying systemic vascular conditions (as hypertension or cardiovascular diseases), which can affect blood flow to the eyes. OPP is defined through the mean arterial pressure (MAP) and the intraocular pressure (IOP), i.e.

$$\text{OPP} = \text{Mean Arterial Pressure (MAP)} - \text{Intraocular Pressure (IOP)}$$

OPP is thought to play a significant role in the pathophysiology of glaucoma. Some studies have identified low OPP as a significant risk factor for the development and progression of glaucoma. However the conclusions of different studies are contradictory, and this is confirmed with the meta-analysis reported in [9].

Our goal is to extend the statistical analysis presented in [8]. In this paper we analyze our data with both frequentist and Bayesian methods. Next, we discuss the results, interpretations and limitations of both methods.

3. Frequentist statistical analysis

Our previous study included descriptive statistics and multiple tests for statistical hypothesis like two sample t-test with equal variances, Welch t-test or Mann Whitney U test, test for distribution of proportions for categorical data as well as logistic regression with Firth correction. The results were presented with p-values without correction for multiple comparison, and where suitable we reported odds ratio, confidence intervals and R^2 . The difference in means of OPP was analyzed with two sample t-test with equal variance and we reported a non-significant p value (0.383). p values were reported without correction for multiple comparisons. OPP was also discussed as a predictor of prevalence of glaucoma.

In this study we discuss and analyze the data for OPP separately from the rest of the dataset. Next, we present results of different

statistical analysis applicable to the dataset. Table 1 gives details on the descriptive statistics.

Table 1: Descriptive statistics on OPP data in glaucoma and non-glaucoma samples.

	Glaucoma (POAG) n=27	Non-glaucoma n=30
Mean:	45.91	47.57
Median:	46.22	47.72
Standard Deviation	7.36	7.71
Min:	32.22	29.67
Max	62.22	67.22

In the conducted statistical tests, H_0 and H_1 stand for the null and alternative hypothesis and are defined in the usual manner. In the case of normality test we test whether the data comes from normal distribution as opposed to the hypothesis that it does not come from normal distribution. Levene's and Student's t-test on the data are two-sided tests. We also calculated the effect size and the power analysis for the t-test. Table 2 summarizes the results.

Table 2: Statistical tests applied on the data set with results

Normality Tests Shapiro-Wilk	Glaucoma (POAG) H_0 vs H_1 p values = 0.99	Non-glaucoma H_0 vs H_1 p values = 0.10
Homogeneity of Variance Levene's Test	H_0 vs H_1 p value= 0.67	
Comparison of Means Student's t-test	H_0 vs H_1 p value 0.38	
Effect Size	Cohen's d D=0.23	
Power Analysis	Power of test 0.14	

With this frequentist analysis we did not reject the null hypothesis that the data is normally distributed in both populations. We support this with the Q-Q plots presented in Fig. 1.

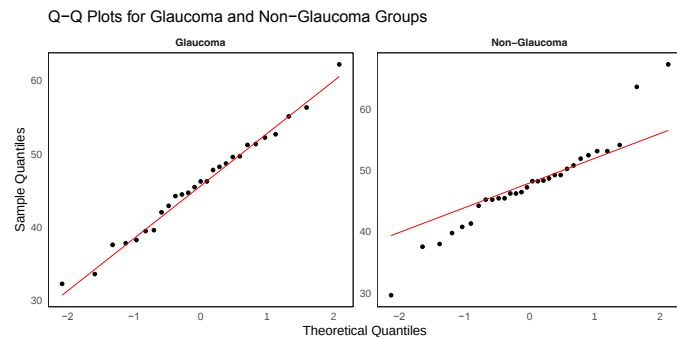


Fig. 1 Normal Q-Q plots of both samples

We also fail to reject the hypotheses that the variances and the means of the two populations are equal. Thus, we state that we did not find a statistically significant difference in OPP between the glaucoma and non-glaucoma groups ($p = 0.38$). The effect size of the t-test is small (Cohen's $d = 0.23$). Cohen's d quantifies the

difference between two group means in terms of standard deviation units and thus it provides a standardized measure of the effect size. The power of the test is low (0.14), suggesting that the sample size may not be sufficient to detect a meaningful difference, if one exists.

Statistical power decreases as the number of statistical tests increases, particularly when using frequentist methods. As the number of tests increases, the sample size for each individual test may become insufficient to detect smaller effects, leading to higher Type II error rates (failing to reject the null hypothesis when it is false). This results in lower power of tests. Thus, further research with a larger sample size is recommended to draw more definitive conclusions. However, this may be an obstacle in medical research, due to financial and time constraints.

We emphasize that many of the studies in the meta-analysis in [9] also reported small sample sizes. Since we can not combine studies, we can not make strong conclusions and decisions. This changes if we apply Bayesian inference. Next, we perform Bayesian analysis for the difference of means of OPP in both groups.

4. Bayesian statistics for hypothesis testing

Bayesian hypothesis testing offers a fundamentally different approach to statistical inference. When using Bayesian methods, we model parameters as random variables with specific probability distributions, rather than fixed values. This allows us to formally incorporate prior beliefs about the parameters and update these beliefs with observed data using Bayes' theorem. The goal is to obtain a posterior distribution, which represents the updated knowledge about the parameters after observing the data.

In our study, we use Bayesian model to assess the difference between the mean of OPP in the glaucoma group μ_g and the mean of OPP in the non-glaucoma group μ_{non-g} . We assume that the data comes from normal distributions with equal variances i.e.

$$y_g \sim N(\mu_g, \sigma)$$

$$y_{non-g} \sim N(\mu_{non-g}, \sigma)$$

The three parameters μ_g, μ_{non-g} and σ are assumed to be random variables and are modeled using some distributions which reflect theoretical and possible prior knowledge about the parameters. We consider three different models:

Model 1.

$$\mu_g \sim U(25,70)$$

$$\mu_{non-g} \sim U(25,70)$$

$$\sigma \sim U(0,10)$$

Model 2.

$$\mu_g \sim N(45,15)$$

$$\mu_{non-g} \sim N(45,15)$$

$$\sigma \sim U(0,20)$$

Model 3.

$$\mu_g \sim N(45,4)$$

$$\mu_{non-g} \sim N(45,4)$$

$$\sigma \sim U(5,12)$$

We assume that both populations have same variances. All three models are partially informed. In the first case, we model both means with uniform distribution on an extended range of the observed data. Together with the assumed distribution of the variance, we get broader assumed distribution for the data.

In the second model we have used prior knowledge obtained from the systemic review and meta-analysis discussed in [9]. We have used the reported values of mean and standard deviation of OPP for both groups to inform the corresponding prior distributions. The priors in Model 3 are more narrow, reflecting the reported data

in [9] while Model 2 allows for more variations. Thus Model 3 is the most dependent on the reported data.

A density plot of the posterior predictive distributions is very helpful for understanding what kind of data can be simulated under the specified model. With the plot we can assess whether the model aligns with our understanding of the data distribution. Fig. 2 represents the plot for the posterior predictive distribution of non-glaucoma data under Model 1. As we can see, most of the simulated data lies in the range [0,100], which is broad from theoretical point of view. The model gives small probability of theoretically extreme values and covers well the theoretically expected values between 30 and 70 for both groups. More details on possible values of OPP in both groups can be found in [9-11].

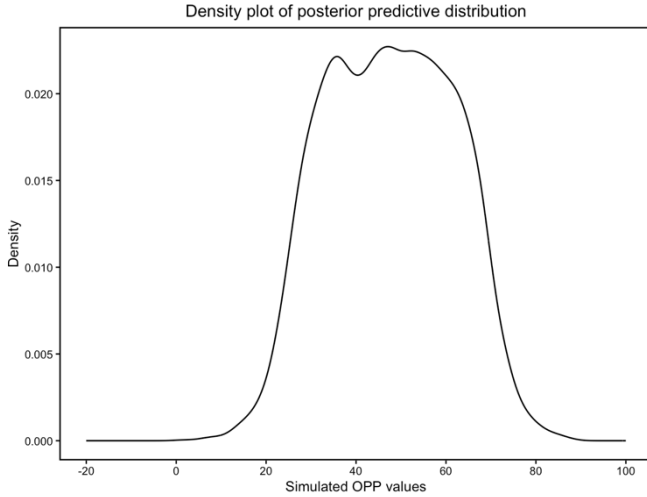


Fig. 2 Density plot for posterior predictive distribution for non-glaucoma data.

For the difference in means $\mu_{diff} = \mu_g - \mu_{non-g}$ we are analysing the two hypotheses

$$\begin{aligned} H_0: \mu_{diff} &= 0 \\ H_1: \mu_{diff} &\neq 0 \end{aligned}$$

Bayesian hypothesis testing directly evaluates the posterior probability of the hypotheses. This involves computing the Bayes factor (BF), a key metric for hypotheses comparison. The Bayes factor is defined as the ratio of the marginal likelihoods of the data under each hypothesis, i.e.

$$BF = \frac{P(data|H_0)}{P(data|H_1)}$$

In this study, we used the Savage-Dickey density ratio which is computationally efficient method to compute the Bayes factor. This method can be applied under specific conditions – the null hypothesis should be a point hypothesis, testing a specific value, which is included in the parameter space of the alternative hypothesis. Thus, the method is suitable for our hypothesis testing. Additionally, the priors used for the parameters must be continuous and proper (i.e., they integrate to 1 over the entire parameter space), which is case with our proposed models. Another assumption, which is needed and fulfilled in our case - the likelihood function under the null and alternative hypothesis must be the same. The only difference between H_0 and H_1 should be the parameter value being tested. Also, the prior for the parameter being tested (in our case μ_{diff}), must be defined in a way that makes it possible to evaluate its density at the null value. More details on Savage-Dickey density ratio can be found in [12].

Under these assumptions the Bayes factor can be calculated as

$$BF = \frac{\text{Posterior density value at } \mu_{diff} = 0}{\text{Prior density value at } \mu_{diff} = 0}$$

To obtain the Bayes factor for each model, we need to simulate data from the corresponding posterior distributions. First we simulate Markov chain Monte Carlo samples for the parameters $\mu_g, \mu_{non-g}, \mu_{diff}$. Next, we need to calculate the value of the prior and posterior density of μ_{diff} at the value 0. In our models, the prior density for μ_{diff} can be obtained explicitly from the chosen priors for μ_{gd}, μ_{non-gd} . The values from the posterior distribution are estimated using kernel density estimate from the MCMC samples of μ_{diff} . The simulations are done using R and JAGS. For more details on MCMC simulations with R and JAGS we refer to [13-15].

Table 3 summarizes the results for the calculated ratio for the three models:

Table 3: Bayes factors for the models

	Savage-Dickey density ratio
Model 1	7.3
Model 2	8.4
Model 3	2.2

Bayes factor with a value greater than 1 is an evidence in favor of the null hypothesis, i.e. the data provides more support for the null hypothesis. As we can see from the table, all three models have values greater than 1. The values are different since they depend on the choice of prior distributions. The most informed prior distributions in Model 3 lead to smallest Bayes factor value, which is less than 3. This is usually considered a weak evidence for H_0 .

5. Discussion of the results and future work

When comparing multiple models we can choose the one that provides stronger evidence for the null hypotheses. Instead of selecting a single model, we can perform Bayesian model averaging, to include the uncertainty in the models. However, given the small sample size, there are few important things to be considered:

- With small sample sizes, the data has limited information. The model with uninformed priors relies more on the observed data, rather than on prior assumptions. This, as in our case, may result in higher Bayes factor which favours the null hypothesis, if the observed data does not show a strong effect. For our study this means the observed difference in means provides more evidence in favour of the null hypothesis.

- Small sample sizes increase the sensitivity to the choice of priors. The informed model may be constrained by the prior information which may yield a lower Bayes factor. The uninformed model is more flexible, leading to a higher Bayes factor.

- The informed priors might be too restrictive – they are based on specific prior knowledge. The prior information overpowers the observed data, and this can lead to a lower posterior density at $\mu_{diff} = 0$, decreasing the Bayes factor in the informed scenario. This issue is amplified when working with small sample sizes.

We emphasize that the models in our study are chosen based on the meta-analysis published in [9]. Complete dataset information is not available and only summarized results for mean OPP are given. The priors may not reflect the true underlying distribution of the

observed data set. Better understanding of the reported studies as well as access to complete datasets will improve the models. Access to complete data sets would be extremely beneficial, allowing validation and reproduction of studies. Additionally, there is need for better understanding of the observed populations and their characteristics in the published studies, including demographic data, age, and sex distribution as well as some characteristic medical variables. Thus, we can decide which data would give the most suitable information for our research. Still, the chosen models help us better understand the given problem.

We also emphasize that many of the studies reported in [9] are based on small samples. These studies cannot interchange their knowledge and use it in their models as we did. A major advantage of Bayesian statistics is that one can continue with collecting data from the populations and create new models based on our current data. This way small sample sizes are not a major drawback, the data sets can be extended, and more reliable conclusions can be made.

The reported values of Bayes factors are not enough to decide for best suited model which we could use for further predictive analysis. Additional sensitivity analysis should be performed, which together with MCMC diagnostics further would ensure the robustness of the analyses. Posterior predictive check is crucial to see how well the model fits the data and this is done by replicating data from the posterior predictive distribution. If the evaluated model fit is poor, we may conclude that the model is missing important aspects of the data, and its conclusions may be unreliable. This would suggest the next steps in the analysis, and we plan to implement these steps in the next stages of our study.

6. Conclusions

In this study we have analyzed data on ocular perfusion pressure in patients with and without primary open angle glaucoma. We have performed both frequentist and Bayesian inference based on Bayes factors and gave interpretation of the results, stressing out the limitations of the dataset and the methods. Better understanding of the models can be obtained by performing posterior predictive check and sensitivity analysis. The models can be improved by historical data as well as enriching the dataset.

Statement by the authors. The work on this paper was partially supported by Faculty of Computer Science and Engineering, University Ss Cyril and Methodius Skopje, Republic of North Macedonia.

References

1. J. P. A. Ioannidis. Why most published research findings are false. *PLoS medicine*. 2.8 (2005): e124
2. A. Gelman, E. Loken. The garden of forking paths: Why multiple comparisons can be a problem, even when there is no “fishing expedition” or “p-hacking” and the research hypothesis was posited ahead of time. *Department of Statistics, Columbia University* 348.1-17 (2013): 3
3. R. S. Nickerson, Null hypothesis significance testing: a review of an old and continuing controversy. *Psychological methods*. 5.2 (2000): 241.
4. D. J. Benjamin et al. Redefine statistical significance. *Nature human behavior*. 2.1 (2018): 6-10
5. E. -J. Wagenmakers, A practical solution to the pervasive problems of p values. *Psychonomic bulletin & review* 14.5 (2007): 779-804
6. J. Vandekerckhove, J. N. Rouder, J. K. Kruschke. Bayesian methods for advancing psychological science. *Psychonomic Bulletin & Review* .25 (2018): 1-4
7. G. Cumming, The new statistics: Why and how. *Psychological science* 25.1 (2014): 7-29
8. G. Dimitrova, A. Ljubic, B. Tojtovska, K. Tagasovska, U. Tomasevic. Pressure Related Ocular Parameters in Caucasian Patients with Primary Open-Angle Glaucoma. *Journal of Ocular Diseases and Therapeutics*. 9, (June 2021), 10-14
9. K. E. Kim, S. Oh, S.U. Baek, et al. Ocular Perfusion Pressure and the Risk of Open-Angle Glaucoma: Systematic Review and Meta-analysis. *Science Reports*, 10, 10056 (2020)
10. M. C. Leske, Ocular perfusion pressure and glaucoma: clinical trial and epidemiologic findings. *Current opinion in ophthalmology*. (March 2009) 20(2):73-8
11. M. C. Leske et al. Risk factors for incident open-angle glaucoma: the Barbados Eye Studies. *Ophthalmology*. 115.1 (2008): 85-93
12. E. J. Wagenmakers et al. Bayesian hypothesis testing for psychologists: A tutorial on the Savage–Dickey method. *Cognitive psychology*. 60.3 (2010): 158-189
13. J. K. Kruschke, "Bayesian analysis reporting guidelines." *Nature human behaviour* 5.10 (2021): 1282-1291
14. J. Van Doorn et al. The JASP guidelines for conducting and reporting a Bayesian analysis. *Psychonomic Bulletin & Review*. 28 (2021): 813-826
15. A. Etz, Q.F. Gronau, F. Dablander et al. How to become a Bayesian in eight easy steps: An annotated reading list. *Psychonomic bulletin & review* 25, (2018): 219-234
16. F.D. Schönbrodt, E.-J. Wagenmakers, M. Zehetleitner, M. Perugini, (2015). Sequential Hypothesis Testing With Bayes Factors: Efficiently Testing Mean Differences. *Psychological Methods*. 22.2 (2017): 322
17. W. Zhengxiao, et al. A review of Bayesian hypothesis testing and its practical implementations. *Entropy* 24.2 (2022): 161
18. R. van de Schoot, S. Depaoli, R. King, et al. Bayesian statistics and modelling. *Nature Reviews Methods Primers* 1, 1 (2021)