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Modeling the Shaking Process of a Walnut Tree: Determining the Natural Vibration Frequency

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Abstract: The results of a study of the shaking process of a walnut tree are presented. Shakers used in harvesting machines are specialized equipment that is attached to the tree trunk and generates controlled vibrations, causing the fruit to fall to the ground or into special catching devices. Thus, universal shakers for various types of nuts, including walnuts, almonds and hazelnuts, ensure fast and uniform harvesting without significant damage to the trees. When harvesting nuts by shaking, the dynamic properties of the trees are important. Therefore, it is necessary to calculate the natural frequency of the system's oscillations, and it plays a key role in the occurrence of the resonance effect. Thus, during the shaking process, the natural frequency of the system includes the tree and other elements interacting with it, which makes it possible to determine the optimal operating modes of the vibrators to ensure the required completeness of fruit removal with the least energy expenditure. For this purpose, the Euler-Bernoulli theory is used, according to which, when solving a dynamic equation for specific fastening conditions, the natural frequencies and corresponding vibration modes are determined, at which the beam oscillates without external forces.

KEY WORDS: OSCILLATION FREQUENCY, SHAKING PROCESS, WALNUT TREE, PHYSICAL MODEL.

Introduction

Harvesting nuts is one of the most important stages in horticultural technology, determining not only the yield of the crop, but also the quality of the final product. Traditional harvesting methods such as manual labor or simple mechanical devices, which are generally labor-intensive and inefficient, are especially ineffective in large orchards or plantations of nut crops such as walnuts, hazelnuts and almonds.

Fruit shakers used in harvesting machines are specialized equipment that is attached to the tree trunk and generates controlled vibrations, causing the fruit to fall to the ground or into special catching devices. As noted by Bradu N., Melnic Iu. et al., mechanized harvesting of nuts provides a solution to the problem of efficient removal of fruits from trees, while reducing harvesting costs to 35-45% of the total cost of production, which ultimately contributes to an increase in overall production efficiency [1, 2, 3]. Compared with manual collection, the use of machines with pulse vibration exciters, mechanized harvesting can increase labor productivity several times [3, 4].

The most common mechanical harvesting system in orchards is shaking the trunks and crowns of trees. As noted by Mohsen Farajijalal et al., the branch shaking system enables selective fruit harvesting due to the varying vibration characteristics of different branches, as well as branches in the tree canopy, depending on their age, water content in the trunk, and elasticity [5]. The morphological characteristics of fruit trees, the diversity of fruit structures, growth patterns and agricultural practices in the orchard are the main factors in choosing the appropriate type of mechanized fruit harvesting system. These basic characteristics will help to select optimal vibration parameters such as frequency, amplitude, duration and type of shaking [4, 5].

Fruit shakers used in harvesting machines are specialized equipment that is attached to the tree trunk and generates controlled vibrations, causing the fruit to fall to the ground or into special catching devices. Thus, universal shakers for various types of nuts, including walnuts, almonds and hazelnuts, ensure fast and uniform harvesting without significant damage to the trees.

Prerequisites and means for solving the problem

Like any other tree, the walnut tree is a complex natural structure and its properties vary depending on the species and age. When harvesting trees, where their dynamic properties are important, it is necessary to calculate the natural frequency of the system's oscillations, since the natural frequency is the frequency at which the system oscillates on its own, without any external influence on it, and which plays a key role in the occurrence of the resonance effect. Thus, during the shaking process, the natural frequency of the system includes the tree and other elements interacting with it, which makes it possible to determine the optimal operating modes of the vibrators to ensure the required completeness of fruit removal.

From the theories of vibrations it is known that vibrations that are supported only by elastic force are called free or natural vibrations, and their frequency depends on the physical characteristics of the tree, such as the length of the trunk, the elasticity of the wood, the mass of the crown, etc. [6, 7]. In this case, the diameter of the cross-section A of the trunk within each section is considered constant and the material is homogeneous. This allows to apply Hooke's law, which states that for elastic deformations (small in magnitude), the normal stress σ in the body is directly proportional to the relative deformation ε , and the proportionality coefficient depends on the properties of the materials – Young's modulus E . In this case, the mass of the crown is brought to a common center of mass, and its interaction with the air is excluded [8].

It has been established that the falling of nuts when the tree is shaken is due to a physical phenomenon known as resonance. If we take into account that resonance is a phenomenon in which an oscillatory system reacts with a maximum oscillation amplitude δ to an external influence, the frequency of which coincides with the natural frequency of the system under study, then this occurs because the external force transfers maximum energy to this system.

In the particular case under study, the tree vibrates at a frequency close to its natural frequency, when the oscillation amplitude δ increases sharply. Therefore, to ensure fruit fall with minimal impact, mechanical shakers should be tuned to a resonant frequency, which will ultimately:

- 1) maximize fruit removal (up to 90–95%);
- 2) minimize damage to the tree trunk and branches;
- 3) reduce energy consumption.

Solution of the examined problem

To calculate the natural frequency of oscillations of a walnut trunk, physical and mathematical models are used to determine the natural circular frequencies for medium and large trunks, as well as the parameters of the rigidity of walnut wood, which are expressed through the expression of Hooke's law [8].

$$\sigma = E\varepsilon \quad (1)$$

where: ε is the relative deformation;

E - Young's modulus, Pa.

It is also formulated as a function of absolute elongation, load, length, and cross-sectional area.

Based on the selected physical model, electronic dynamometers connected to a computer are used in practice to determine the frequency of free oscillations or natural frequency.

The trunk is usually modeled as a cantilevered cylinder, rigidly fixed at the base and free at the end (top). For this purpose, the Euler-Bernoulli theory is used, according to which, when solving a dynamic equation for specific fastening conditions (for example, clamping), the natural frequencies and corresponding vibration modes are determined, at which the beam oscillates

without external forces. It should be noted that the theory is most accurate for thin beams and small deformations. For short and thick beams or large deformations, more complex theories are required that take into account shear deformations and nonlinear effects.

Results and discussion

To perform calculations, it is necessary to adopt a calculation scheme, the physical model of which is presented in Fig.1. A real trunk is not perfectly uniform, usually spherical and less commonly conical. Root rigidity may not provide sufficient anchorage, which reduces the oscillation frequency. Branches and foliage on trees during harvesting increase their effective mass and also reduce the oscillation frequency f (Fig.1,b).

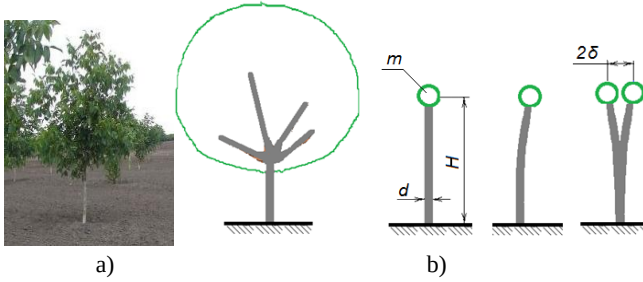


Figure 1. Physical model for determining the frequency of free oscillations: a) walnut tree; b) physical model; H – height of the tree; d – trunk diameter; m – nominal mass; δ – amplitude of vibration.

If in the calculation scheme there is a concentrated mass m at the top of the rod (fruits, branches, leaves), then it is necessary to take into account the reduced mass (the usual correction), since with a large mass m the oscillation frequency f decreases.

The mathematical model for such a homogeneous cantilever beam of circular cross-section with diameter d expresses the natural angular frequencies ω_n (rad/s) in the following form [6, 7]:

$$\omega_n = \beta_n^2 \sqrt{\frac{EI}{\rho A l^4}} \quad (3)$$

where: β_n are the coefficients of n modes of natural oscillations;

I – moment of inertia of the section, m^4 ;

ρ – bulk density of the trunk, kg/m^3 ;

A – cross-sectional area of the trunk, m^2 ;

$l=H$ – reduced length of the trunk or height of the tree, m.

In this case, Young's modulus for walnut wood is taken to be within the range of 8.0-14.0 GPa, depending on the variety, humidity and direction of the walnut wood fibers [8].

Since the mass of the tree is distributed along the trunk, according to the Euler-Bernoulli theory, there are n modes of natural oscillations [6, 7]. In formula (3), the coefficients β_n (the first three) are standard numbers:

$$\beta_1 \approx 1.9, \beta_2 \approx 4.7, \beta_3 \approx 7.9, \dots$$

When solving a dynamic equation for specific fastening conditions (for example, clamping), the natural frequencies and corresponding vibration modes are determined, at which the beam (trunk) vibrates without external forces.

It should be noted that the theory is most accurate for thin beams and small deformations. For short and thick beams or large deformations, more complex theories must be used that take into account shear deformations and nonlinear effects [8, 9, 10].

Then the natural frequency f_n of the trunk expressed in hertz (Hz) is equal to:

$$f_n = \frac{\omega_n}{2\pi} \quad (4)$$

In practice, shaking of a walnut tree trunk occurs at the first fundamental frequency ($n=1$), because under real-world conditions, it is the one that manifests itself most strongly. Then, expression (3) takes the following form:

$$\omega = \omega_1 = \beta_1^2 \sqrt{\frac{EI}{\rho A l^4}} \quad (5)$$

$$\text{or simplified} \quad \omega = \beta_1^2 \sqrt{\frac{EI}{\rho A l^4}} \quad (5,a)$$

where $\beta_1 \approx 1.9$.

As a first example, we take an average trunk of a walnut tree with the following parameters:

- Young's modulus $E=11.0$ GPa;
- trunk diameter d takes values from 0.15 to 0.3 m;
- reduced length of the trunk or height H of the tree takes values from 4.0 to 8.0 m;
- bulk density of the trunk $\rho=650$ kg/m^3 .

First, the cross-sectional area of the trunk A is determined using the formula:

$$A = \frac{\pi d^2}{4} \quad (6)$$

The moment of inertia I of a circular cross-section is determined by the formula:

$$I = \frac{\pi d^4}{64} \quad (7)$$

Substituting the corresponding values of the parameters of the walnut tree trunk into formulas (6) and (7), we obtain the values of the cross-sectional area A of the trunk and the moment of inertia I of the circular cross-section, respectively.

$$\omega = \beta_1^2 \frac{d}{4l^2} \sqrt{\frac{E}{\rho}} \quad (8)$$

Taking into account formula (4), the natural frequency f_n of the the trunk, expressed in hertz (Hz), is equal to:

$$f = \beta_1^2 \frac{d}{8\pi \cdot l^2} \sqrt{\frac{E}{\rho}} \quad (9)$$

After calculating the natural angular frequency ω using formula (5,a) and the natural frequency f_n , expressed in hertz, using formula (4), the calculated data are summarized in Table 1.

Table 1. Natural frequency of a walnut tree trunk

Trunk parameters		Geometric characteristics of the section		Natural angular frequency of oscillations ω , rad/s	Oscillation frequency f , Hz
Diameter d , m	Height H , m	Cross-sectional area A , $\cdot 10^{-2} m^2$	Moment of inertia of a circular cross-section I , $\cdot 10^{-5} m^4$		
2	2	4	5	6	7
0.15	4.0	1.77	2.48	34.74	5.53
	5.0	1.77	2.48	22.22	3.54
	5.5	1.77	2.48	18.37	2.93
	6.0	1.77	2.48	15.44	2.46
0.20	5.0	3.14	7.85	29.68	4.73
	5.5	3.14	7.85	24.54	3.91
	6.0	3.14	7.85	20.64	3.29
	6.5	3.14	7.85	17.57	2.80
0.30	5.0	7.10	39.74	44.45	7.08
	5.5	7.10	39.74	36.73	5.85
	6.0	7.10	39.74	30.87	4.92
	6.5	7.10	39.74	26.31	4.19
	7.0	7.10	39.74	22.69	3.61
	8.0	7.10	39.74	17.35	2.76

From the analysis of the data from Table 1 it follows that, with the same diameter of the trunk of a walnut tree, as its height increases, the natural frequency of oscillations of the trunk decreases (Fig.2). However, for the same tree height, the natural

frequency of trunk vibrations increases with increasing trunk thickness (Fig.2). For example, with a conventional height of the trunk of a walnut tree $H=5$ m, the frequency of natural f oscillations of the trunk will be equal to 3.54 Hz for a diameter of $d=0.15$ m, 4.73 Hz for $d=0.20$ m, and 7.08 Hz for $d=0.30$ m.

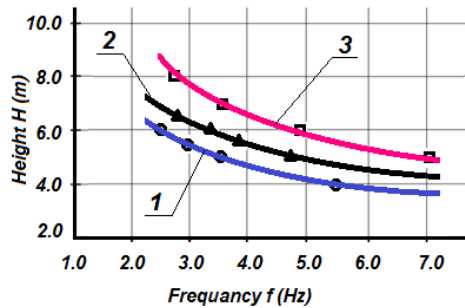


Figure 2. Dependence of natural frequency f of oscillations on the height H of the trunk: 1 - $d=0,15$ m; 2 - $d=0,20$ m; 3 - $d=0,30$ m.

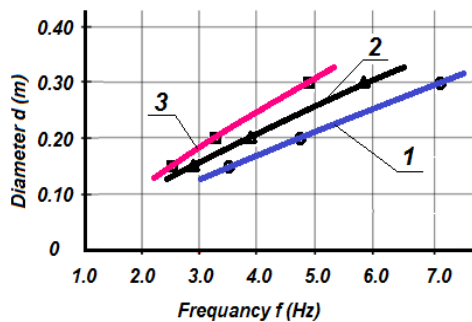


Figure 3. Dependence of natural frequency f of oscillations on the diameter d of the trunk: 1 - $H=0,50$ m; 2 - $H=0,55$ m; 3 - $H=0,60$ m.

From formula (9) we determine the diameter d of the trunk:

$$d = \frac{8\pi \cdot H^2 f}{\beta_1^2} \sqrt{\frac{\rho}{E}} \quad (10)$$

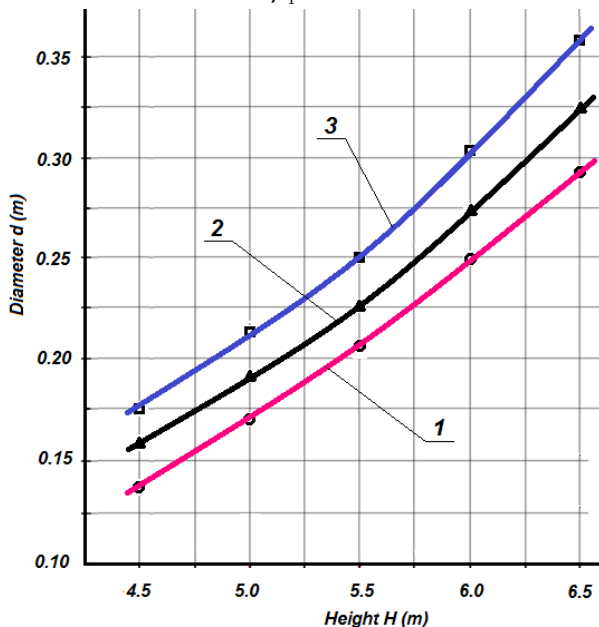


Figure 3. Dependence of the height H of a walnut tree on the diameter d of the trunk at fixed vibration frequencies f : 1 - $f=4,0$ Hz; 2 - $f=4,5$ Hz; 3 - $f=5,0$ Hz.

Figure 4 shows the dependence of the height H of a walnut tree on the diameter d of the trunk at fixed vibration frequencies f . It means that if, for example, we initially set $f=5$ Hz, i.e. $f=5$ oscillations per second, then in order to maintain this parameter, we

need to selectively measure the trunk diameter of several trees in the garden and to determine its arithmetic mean value d_m . The graph in Fig.4 can be used as a nomogram to set the tree height H to be the same for all trees in a nut orchard for the next year, taking into account the annual growth rate of branches and determining the working height for adjusting the machine during mechanized pruning of the orchard. For example, for a trunk diameter $d_m=0.24$ m and an oscillation frequency $f=5$ Hz, according to the nomogram, the height of the trees should be equal to $H_m=5.35$ m (Fig. 4).

Conclusions

1. Modeling the process of shaking a walnut tree made it possible to obtain the dependence of the natural frequency of oscillations f of the tree on the trunk diameter d and on the height of the tree in the range of 0.15-0.30 m and 4.0-8.0 m, respectively. The obtained results show:

- for a walnut tree with the same trunk diameter d , as its height increases, the frequency f of oscillations of the trunk decreases;
- for the same tree height H , the natural frequency of trunk oscillations f increases with increasing of thickness of the tree d .

2. The graph in Figure 4 can be used as a nomogram to set the tree height H to be the same for all trees in a nut orchard for the next year, taking into account the annual growth rate of branches and determining the working height for height adjustment during mechanized pruning of the orchard.

3. Tuning the shakers to the resonant frequency of the tree promotes higher-quality collection of nuts with minimal effort required to break the nut off.

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Study on the dynamics of truck loader crane during cargo unloading using modeling and simulations

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Abstract: This article is a study on the work operation of a hydraulic crane installed on a heavy truck known as Truck Loader Crane. The crane is used to carry loads from the truck to the ground and vice versa. It usually is an integral part of the truck mounted behind the cabin or behind the cargo body, and there are cases when it is additionally mounted on the truck. The crane has several mechanical and hydraulic parts. It is controlled from the command panel attached to the crane or by using the remote panel. The work operation analyzed is cargo unloading from the truck body on the ground. It is a complex process consisting of attaching the cargo (load) to the boom, lifting the cargo from the truck body, transferring the cargo several meters, and lowering it on the ground. During this process, the crane undergoes heavy oscillations due to the motion and swinging of the load it carries. The type of analysis is dynamic analysis, and the methodology consists of 3D modeling of the crane and implementing simulations with SimWise4D software. Through this study, the aim is to identify the nature and extent of forces and stresses on the crane and its parts, the intensity of the swinging and oscillations of the cargo, and their effect on crane operation. High oscillations can cause parts failure and raise concerns about safety. Results will be shown in graphical form for the main influential parameters. Conclusions from this paper will be useful regarding the strength of crane materials, motion dynamics and motion control of crane and cargo, design of crane parts and safety during work. The Truck Loader Crane model is designed based on the data from the standard manufacturer.

Keywords: TRUCK LOADER CRANE, CARGO UNLOADING, OSCILLATIONS, DYNAMIC ANALYSIS, MODELING, SIMULATIONS

1. Introduction

The crane that will be studied is shown in Fig.1. It is a hydraulic type crane mounted on the heavy truck. The study example is from a local company in Prishtina City that handles transport of pallets and other loads. There are two main work activities of the Crane:

- Lifting the load from the ground and lowering it to the truck's cargo body.
- Taking the load from the truck and lowering it to the ground, to some platform or even to a certain height, depending on the request.

There are situations when the crane keeps the load steady at a certain height to stabilize it for a certain amount of time.

The height H of lifting is around 2 – 3 m from the ground, depending on the cargo (load) dimensions. Crane has a defined lifting velocity.

The cargo (load) can be in various forms, it is usually a pallet with various materials, various boxes, concrete structures – pipe or plate, metallic structures, cylindrical form material, etc.



Fig.1. Crane mounted on the truck in the working environment

The type of crane is Palfinger PK 11001 [1], [3], with maximum lifting capacity $Q = 4000$ kg. It is mounted on a Mercedes Benz 1317 heavy truck (Fig.1). Main technical data are taken from the manufacturer's manuals and notes placed on the crane, which are shown in Table.1.

Table.1. Technical features of the Palfinger Loader Crane [1]

Crane Specifications	
Model	PK 11001
Capacity-max	4000 kg to 2.5 m range
Capacity-min	340 kg to 18.8 m range
Load torque	109 kNm
Max manual outreach	23.4 m
Max hydraulic outreach	15 m
Slewing angle	420 °
Operating pressure	290 bar
Dead weight	1510 kg

The main parts of the crane are presented in Fig.2.

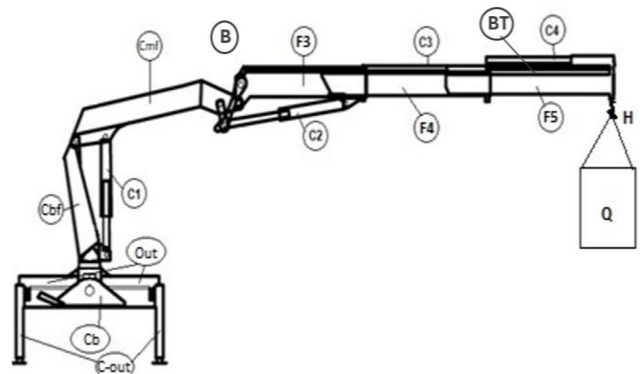


Fig.2. Crane parts: **Out**-Outriggers; **C-out**- Outrigger cylinders; **Cb**- Crane base; **Cbf**- base frame, **B**- Boom with frames; **Cmf**- Middle frame; **F3, F4, F5** – Crane upper frames (beams), **C1, C2, C3, C4** – Crane cylinders; **BT**-Telescopic Boom; **Q** – Load (cargo); **H** – Hook [4]

An electro- hydraulic system is used to move the crane. After the lifting command from the panel, the hydraulic oil is delivered by the gear pump to the oil cylinders, which pushes upwards its pistons. Then, the pistons move the Boom and load Q in various directions (Fig.2).

Dimensions of the cargo body of Mercedes Truck are Length: 7.3 m, width: 2.3 m. Cargo body of the truck is 1.5 m up from the ground.



Fig.3. Rear view foto of the main Crane Parts

Results of the research will be acquired for some main parts of the crane. Forces, torque, stresses and oscillations of the cargo-load during the cargo lowering from the truck body to the ground are considered main influential parameters for measuring strength and strain of crane [4], [5], [6]. The analysis will be carried out for the cargo-load capacity $Q = 1500$ kg, which is the lifting capacity for the crane based on the crane specifications and Load Q carrying distance that will be around 7 m [1]. Maximal motion speed of the crane can reach $v_{cmax} = 0.7$ m/s. Results will be presented with graphs and then discussed.

Regarding the Literature review, some authors in their papers have studied Truck loader cranes, shown in the References, with studies regarding the crane dynamic analysis [4], [5], [7], modelling [5], [8], [11], simulations [5], [6], [11], [12], theory of dynamic analysis [7], [12], motion control and regulation [6], [9], [10] and crane safety [13].

2. Modeling of the Truck Loader crane and simulations scenario

Modell of the Truck Loader Crane is designed with software SimWise 4D [2]. The model contains Mercedes Truck and Loader crane with its important parts, Basement and Load Q .

Working load Q as a cargo to be carried has a box form with dimensions: *Length* = 1 m, *Width* = 1 m, *Height* = 1 m, *Mass* $Q = 1500$ kg. It is placed on the Truck cargo body, ready to be moved. (Fig.4).

Loader crane has its outriggers extended for stability purposes. Distance of the outrigger from Crane Base is 2.1 m.

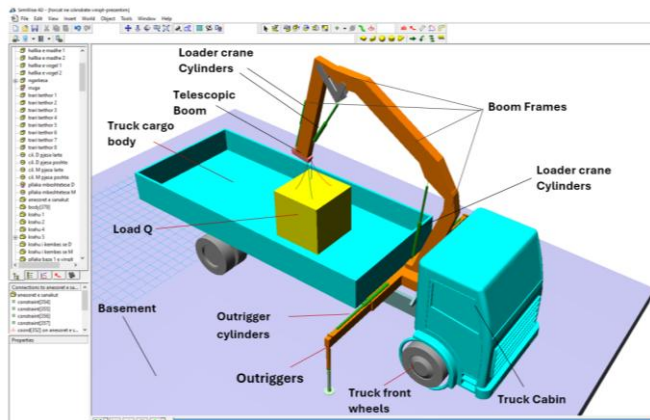


Fig. 4. Model of the Truck and Loader Crane with main parts in the software environment, in the initial position [2]

After completion of the model, simulations will be carried out to get results. Analysis with simulations will be acquired using two numerical Methods, namely Finite Elements Method (FEM) and Numerical Kutta-Merson Method, which are part of the software modules.

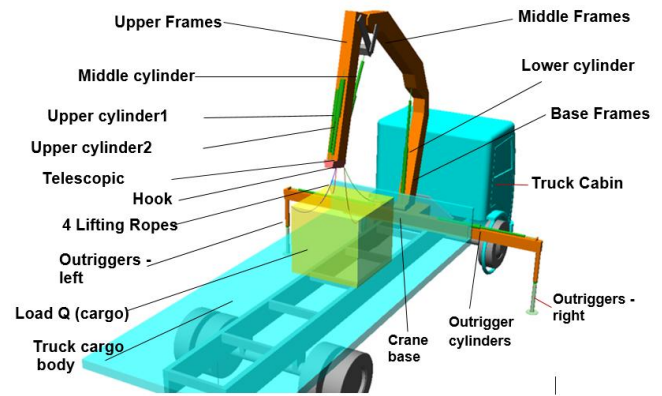


Fig.5. Modelled main parts of the Crane mounted on the truck (Rear view)

For the proper analysis of the load lowering, simulations will be organized as close as to real occasions [6]. The plan is to unload the load Q in the distance around $D = 7$ m from the Crane base (center). This distance is selected randomly. There are five phases of continuous Crane and Load motion identified:

- *Phase 1:* The Crane's Boom in its initial position is linked with the Load Q through the Hook and the Lifting ropes, which are not restrained (loose). Load Q stands on the cargo body at the height of 1.6 m from the ground. (Fig.4 & Fig.5).

- *Phase 2:* Crane cylinders will start the lifting from the time $t_1 = 0$ s. Initially, they will lift unrestrained 4 ropes, and then the Load Q . Lifting will continue slowly, until the height of load 2.23 m from the ground, until the time $t_2 = 5$ s.

- *Phase 3:* Next motion is Right turning of the Boom with load Q , until time $t_3 = 21$ s. The time is longer in order to minimize the excessive load swinging.

- *Phase 4:* In this phase is the horizontal extension of Telescopic Boom and upper cylinders with load Q , to reach the unloading position in final the distance $D \approx 7$ m. During this phase, the load moves horizontally to the right direction. This phase lasts until time $t_4 = 40$ s.

- *Phase 5:* In this phase is the lowering of the load on the ground. It lasts until the time $t_5 = 43$ s. This is the final motion process when the load Q is unloaded on the ground (Fig.6).

After the time $t_5 = 43$ s there is no motion, but the simulation will continue until the time $t_s = 47$ s to monitor the occurrences on the crane after the end of the load motion [6].

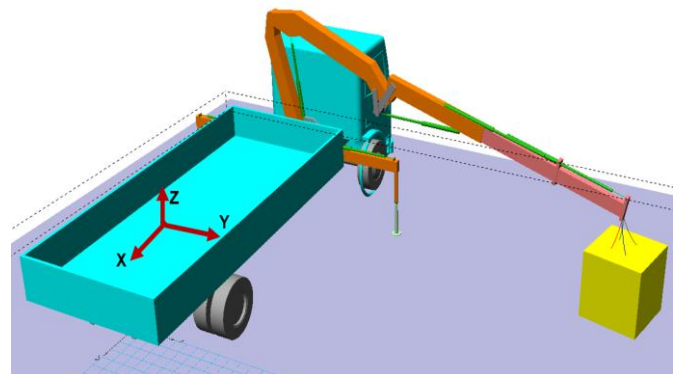


Fig.6. Final position of the simulation - Load Q is unloaded on the ground

3. Results of the unloading

Results of the Load motion and unloading will be presented in the form of graphs for influential dynamic parameters for some main parts of the crane and for the load Q . These parameters are kinematic and dynamic in nature: Forces in the cylinders, Resultant Force and Torque in joints, Stress in the crane frame; Load Q motion, speed and swinging.

3.1. Force in the Cylinders

There are four cylinders in the Boom Frames of the Loader crane that will be analyzed (Fig.7). The parameter that will be measured is the force in the pistons of the cylinders while moving the load. The nature of this force is pressure force.

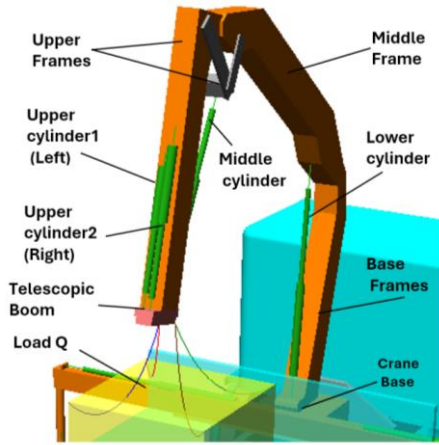


Fig.7. View of the Boom cylinders

- *Force in the Lower Cylinder.* In Fig.8 is the graph of the Pressure force F_{p1} in the piston of the lower cylinder. This cylinder is connected on the bottom side with the Crane Base and on the upper side with a Middle frame. Based on the graph, the piston of this cylinder is heavy loaded part. The force has negative values, while it is a pressure force.

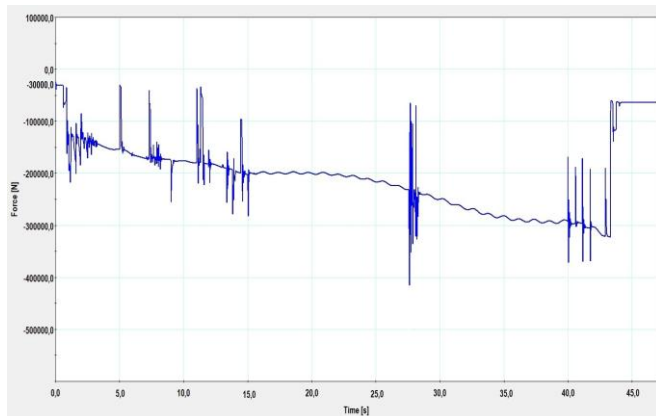


Fig. 8. Force on the piston of the Lower Cylinder

Based on the graph Fig.8, at the start of the lifting, piston force is smaller, around $F_{p10} \approx -30000$ N. On time $t = 1$ s it reaches the value $F_{p11} \approx -130000$ N. With the continuation of the lifting process, until time $t = 14$ s, the piston force increases up to $F_{p12} \approx -200000$ N. Between the time $t = 14$ s until $t = 22$ s the intensity of force does not change significantly, almost constant, with some oscillations. This is the time when cylinder holds steadily the lower and middle frame, while other cylinders move the upper frames with the load Q. Next, between the time $t = 22$ s until $t = 43$ s the value of force is increasing up to $F_{p13} \approx -320000$ N. On time $t = 43$ s the load is lowered on the ground. The piston force decreases significantly, to the value of $F_{p14} \approx -65000$ N, while it carries only the weight of the frames and Telescopic Boom of the crane.

During the entire process, the piston is heavily loaded with pressure force, with high oscillations that result in intense amplitudes. In some moments of the process, there are short timed high jumps of force values as a result of intense oscillations. These are particularly present at the start of the process, between the time $t = 1$ s $\div$ 3 s, between the time $t = 27$ s $\div$ 28 s and $t = 40$ s $\div$ 43 s.

- *Force in the Middle Cylinder.* In Fig.9 is the graph of the Pressure force F_{p2} in the middle cylinder. This cylinder is connected on one side with the Middle Frame and on another side with upper frame. Based on the graph, the piston of this cylinder is also heavily loaded part. At the start of the lifting, piston force is around $F_{p20} \approx -7000$ N. On time $t = 1$ s it reaches the value $F_{p21} \approx -50000$ N. During the lifting process, until the time $t = 14$ s, the piston force increases up to $F_{p22} \approx -110000$ N. Also in this cylinder, between the time $t = 14$ s until $t = 22$ s the intensity of force is almost constant, but with some oscillations. Next, between the time $t = 22$ s until $t = 43$ s the value of force increases up to $F_{p23} \approx -225000$ N. After time $t = 43$ s, the load is lowered on the ground, so the piston force decreases significantly, to the value of $F_{p24} \approx -28000$ N, while it carries only the weight of the Upper frames of the crane.

For this piston, the conclusion is that it is heavily loaded with pressure force during the entire process, but with less intensity of the force compared with Lower cylinder. There are high oscillations that result in intense amplitudes. In addition, there are short timed high jumps of force values because of intense oscillations.

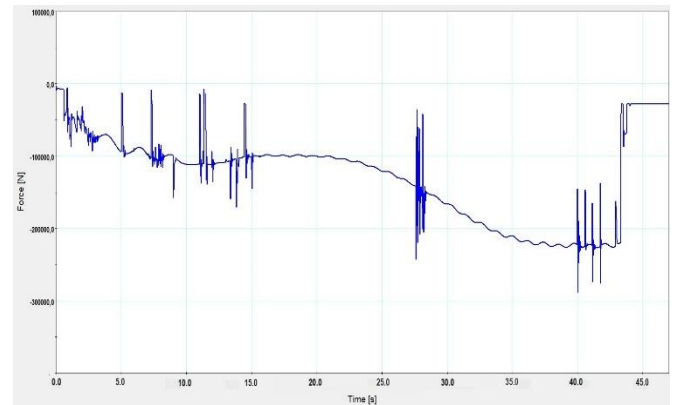


Fig. 9. Force on the piston of the Middle cylinder

- *Force in the Upper cylinder1.* In Fig.10 is the graph of the Pressure force F_{p3} in the upper cylinder 1 (left) (Fig.7). This is one of the two cylinders connected with Telescopic Boom used mainly to push or pull the load Q. Based on the graph, the piston of this cylinder is also heavily loaded part, but with less intensity of the force compared with two previous cylinders.

At the start of the lifting, piston force is around $F_{p30} \approx 2500$ N. It is a push force, has a positive value, while the cylinder is pushing the telescopic Boom. On time $t = 1$ s it reaches the value $F_{p31} \approx 16500$ N. During the pushing process, until the time $t = 14$ s, the piston force drops to $F_{p32} \approx -800$ N. Between the time $t = 14$ s until $t = 41$ s the intensity of force is almost constant, around $F_{p33} \approx -800$ N, but with oscillations in form of sinusoids. After time $t = 43$ s, the load is lowered on the ground, so the piston force decreases up to $F_{p34} \approx 500$ N, carries no load.

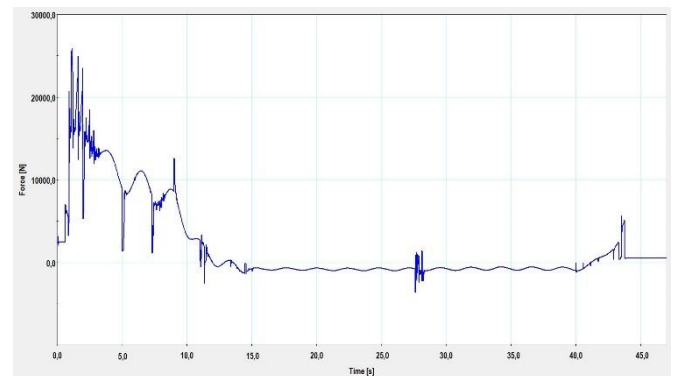


Fig. 10. Force on the piston of the Upper cylinder 1 (left)

- *Force in the Upper cylinder2.* In Fig.11 is the graph of Pressure force F_{p4} in the Upper cylinder 2 (right) (Fig.7). This is the second of the two cylinders pushing the Telescopic Boom, used mainly to

push and pull the load Q . The piston of this cylinder is also heavy loaded part, but with less intensity of the force compared with the first two cylinders.

Based on the graph, there are similarities of the piston force in this cylinder compared to Upper Cylinder 1, in terms of intensity and oscillations.

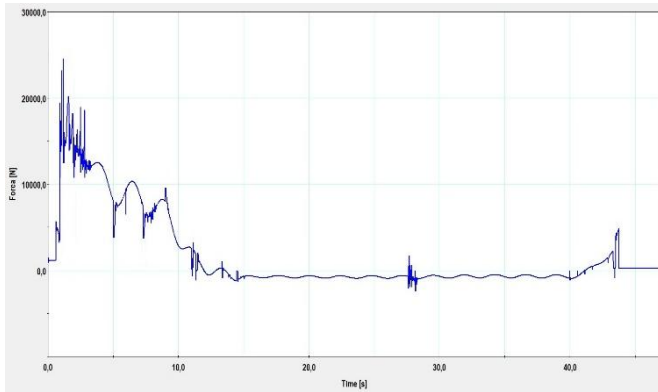


Fig. 11. Force on the piston of the Upper cylinder 2 (right)

3.2. Forces in connections (joints)

Connections or joints between crane parts are heavily loaded parts. There can be different types of connections in form of joints that represent the connection between parts in the form of restraints. Typical types can be Rigid joints, Revolute joints, Rigid Joints on slot, etc. We will present one significant joint between main parts of the crane Connection-joint between Crane Base and Base frame (Fig.12). It is a type of Revolute joint.

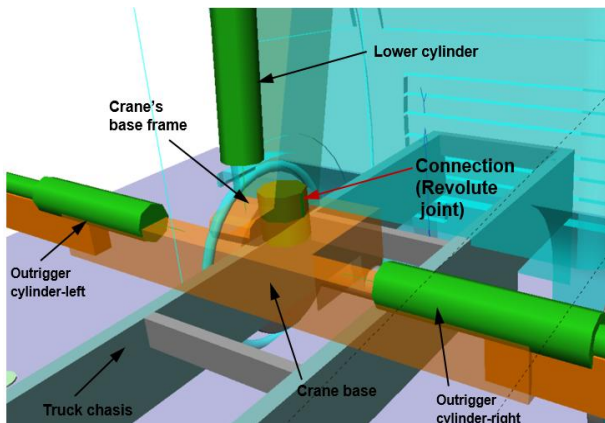


Fig.12. Connection-joint between Crane Base and Base frame

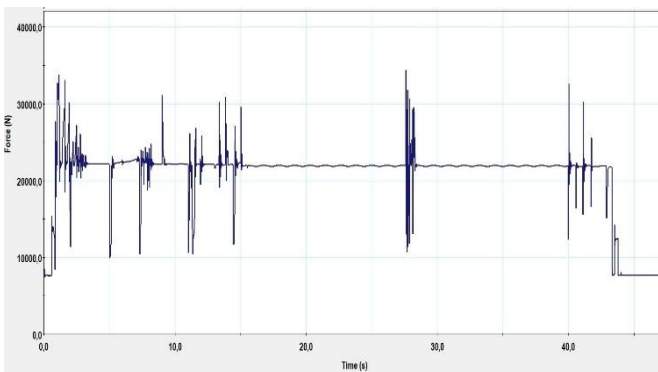


Fig. 13. Force in the connection between Crane Base and Base frame

In Fig. 13 is given the graph of Resultant Force F_{r1} in the connection. At the start of the lifting, resultant force is smaller, around $F_{r1} \approx 8000$ N. The medium value of this force for entire

process is $F_{rm} \approx 22500$ N. At the end of the motion, after the Load is unloaded on the ground the Resultant force drops significantly, around $F_{r1} \approx 8000$ N. There are short timed high jumps of Resultant force values because of intense oscillations. These are particularly present at the start of the process, between the time $t = 1$ s ÷ 2.5 s and repeat several times during the process. Conclusion is that this connection is heavily loaded with reaction force and with oscillations in entire motion process.

In Fig. 14 is the graph of resultant torque (Force moment) in the joint. At the start of the lifting, torque is small, around $T_1 \approx 11000$ Nm. On time $t = 1$ s it reaches the value $T_2 \approx 50000$ Nm. With the continuation of the lifting process, until time $t = 12$ s, the torque increases up to $T_3 \approx 80000$ Nm. Between the time $t = 12$ s until $t = 22$ s the value of torque does not change significantly in intensity, but has oscillations. Next, between the time $t = 22$ s until $t = 43$ s the value of torque is increasing up to $T_4 \approx 119000$ Nm. There are also short timed high jumps of torque values as a result of intense oscillations. After time $t = 43$ s, when the load is lowered on the ground, the torque decreases significantly up to the value of $T_1 \approx 20000$ Nm, while it carries only the weight of the frames and Telescopic Boom.

We can conclude that this joint (connection) is heavily loaded during the entire process, with high oscillations that also result in intense amplitudes.

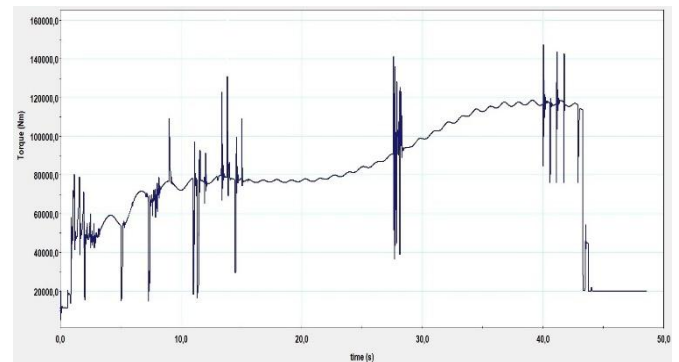


Fig. 14. Torque in the joint – connection between Crane Base and Base frame

3.3. Motion and Speed of the Load Q

In this paragraph will be presented the motion of the Load Q, its swinging and oscillations, and its speed. In Fig.15 is given the movement trajectory of the Load Q in three axes of directions, based on coordinate system shown in Fig.6. According to the curves of the graph in Fig.15, we can see the motion trajectory and swinging of the Load Q.

Note: The position of Load Q represents the position of its Center of mass, which is 500 mm (0.5 m) inside from its edges.

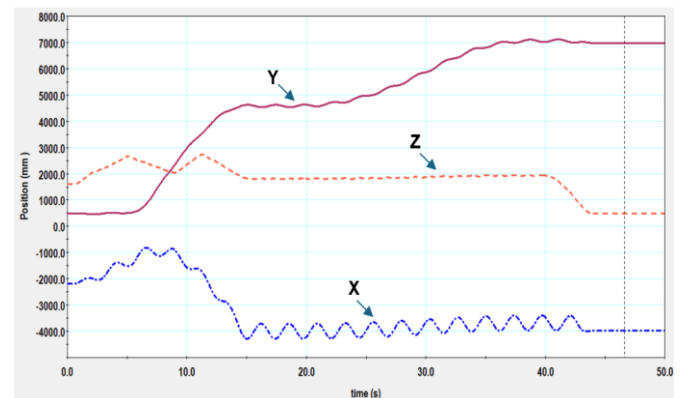


Fig. 15. Position and motion of the Load Q (mm).

The trajectory towards Y axis, in red color, full line, shows the motion in the right direction and starts from initial position of $Y = 500 \text{ mm}$ to the final distance $Y \approx 7000 \text{ mm}$ (7 m). Between $t = 0 \text{ s}$ and $t \approx 6 \text{ s}$ there is no motion towards Y axis (flat line), while during this time there is a vertical lifting of the load towards Z axis and some oscillations towards X axis. Between time $t \approx 6 \text{ s}$ and $t \approx 15 \text{ s}$ there is a rotation of the load to the right, and after time $t \approx 15 \text{ s}$ there is a horizontal motion of the Load Q in the right direction.

Trajectory towards Z-axis, in orange color, dashed line, shows vertical motion of the Load Q. It starts from initial position of $Z = 1600 \text{ mm}$ to the final distance on the Ground $Z \approx 500 \text{ mm}$. Between time $t = 15 \text{ s}$ and $t \approx 40 \text{ s}$ there is no vertical motion towards Z axes (flat line), while during this time there is only horizontal motion of the load Q.

Trajectory towards X axis, in blue color, dash-dot line, shows the motion that starts from initial position of $X = -2000 \text{ mm}$ to the final position $X \approx -4000 \text{ mm}$. Based on this curve, the load has intense swinging and oscillations towards X axes at entire motion process. The amplitudes of swinging can be up to $A_L \approx 300 \text{ mm}$.

In Fig.16 is given the Resultant Speed of the Load Q. Based on the speed curve we can conclude that load undergoes intense oscillations of the motion speed at entire process. Highest amplitudes of speed appear on times $t = 2 \text{ s}$ to $t = 15 \text{ s}$ which is the process of lifting and rotation of the load Q. Maximal value of the speed is $v_{\max} = 1.23 \text{ m/s}$ at time $t \approx 14 \text{ s}$. After the time $t = 15 \text{ s}$ the oscillations of resultant speed have lower intensity, almost same amplitudes but high frequencies, and continue until the end of the motion $t_{\text{end}} = 43 \text{ s}$, when the load Q is lowered on the ground.

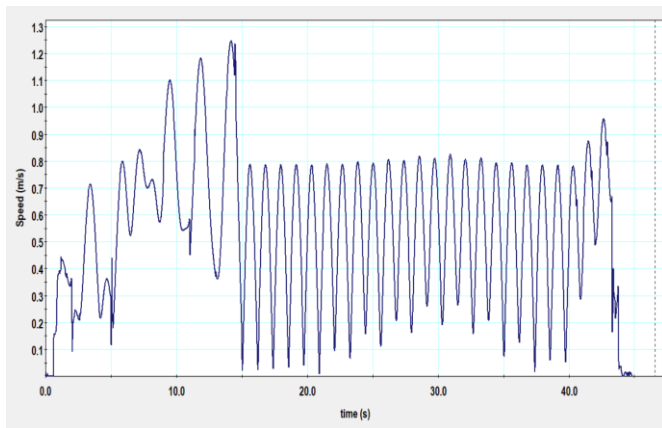


Fig. 16. Resultant speed of the Load Q (mm/s).

3.4. Stress on the Crane frame

We will present the stress of one part of the Crane that is heavily loaded, the Base frame. The type of stress is Von Misses stress. In Fig.17. is given the graph of stress.

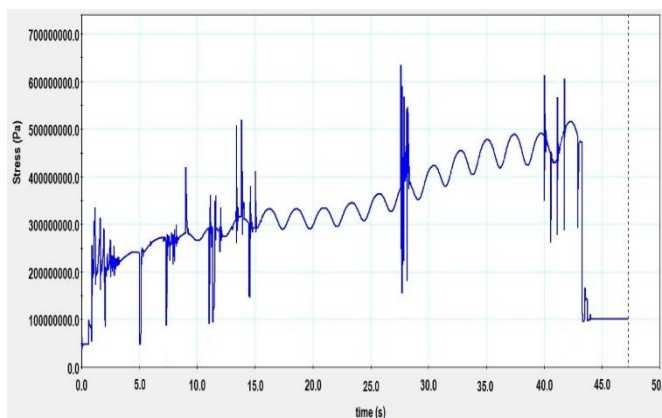


Fig. 17. Graph of Stress on the Base Frame of the Crane Boom (Pa)

Based on the graph Fig.17, at the start of the lifting, stress on the Base Frame is around $\sigma_0 \approx 50000000 \text{ Pa} = 5 \cdot 10^7 \text{ Pa}$. On time $t = 1 \text{ s}$ it reaches the value $\sigma_1 \approx 2 \cdot 10^8 \text{ Pa}$. Until time $t = 14 \text{ s}$, the Stress increases up to $\sigma_2 \approx 3.15 \cdot 10^8 \text{ Pa}$. Between the time $t = 14 \text{ s}$ until $t = 22 \text{ s}$ the intensity of Stress does not change significantly and has heavy oscillations. Between the time $t = 22 \text{ s}$ until $t = 43 \text{ s}$ the value increases up to $\sigma_3 \approx 5.15 \cdot 10^8 \text{ Pa}$.

After time $t = 43 \text{ s}$, when the load is lowered on the ground the value of stress decreases significantly, to the value of $\sigma_4 \approx 1 \cdot 10^8 \text{ Pa}$, while it carries only the weight of the frames and telescopic Boom of the crane.

Conclusion is that Base frame is heavily loaded part with dynamic stress in entire motion process. Also, based on Fig.19, there are short timed high jumps of stress values as a result of intense oscillations. These stress value jumps are a matter of concern regarding material durability, while in short time and in some periods of motion, it can exceed the tensile stress of the material [13].

In Fig.18 is shown an example of stress dispersion in the Base frame on its entire volume, in the time $t \approx 14 \text{ s}$. The part is meshed and calculated using Finite Elements Method (FEM). Based on the color contrast on the volume, the values of stress are not equally dispersed. Maximal values of stress are in the lower part, at the joint between the Base frame and Crane base.

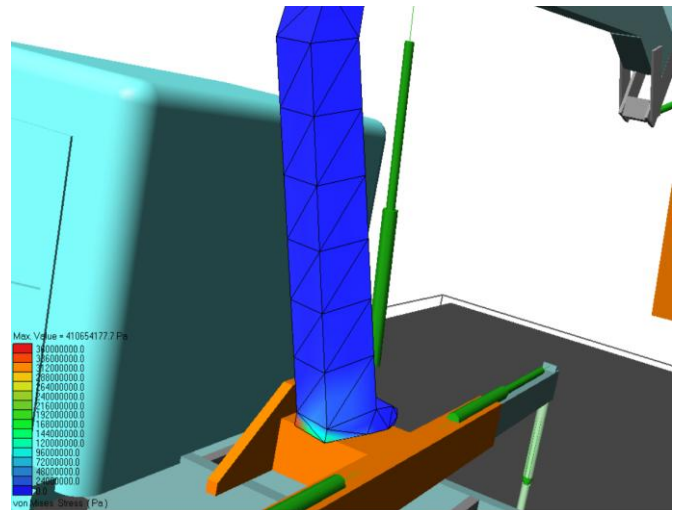


Fig. 18. Sample of dispersion of the Stress on the Base Frame in the time moment $t = 14 \text{ s}$

4. Conclusions

In this study, we analyzed lowering of the load by the Truck Loader crane and analyzed the dynamics of this work operation. Analysis was focused on some main parts of the Loader crane: Main frames of the Boom, cylinders that move the boom frames and the load, main joint in crane base and motion of the Load Q.

Based on the analysis and results, we can conclude that during the load lowering the crane is heavily loaded with dynamic occurrences and oscillations that are present on entire duration of the process. Matter of concern are some temporary jumps of forces, torque intensity and stresses during the motion that can be short in time, but with high values. This can lead to safety issues; therefore, it is important to have slow speed of the Load Q. In addition, the motion needs to be controlled so that the Load Q does not swing and oscillate heavily, which can lead to problems in the crane and truck stability.

The dynamic parameters selected for analysis best represent the dynamics of the motion, and these are forces, torque, stresses and the motion of the Load Q. Results of the parameters are shown in graphical form and discussed, and conclusions are given for each case.

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CFD and Differential Evolution Optimization of an Air-To-Air Heat Recovery System for an Industrial Dryer

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Abstract: This study details the thermal and fluid dynamic performance analysis and geometric optimization of a compact plate heat exchanger designed for waste heat recovery in industrial drying systems. The objective is to preheat fresh process air (25°C) to a target temperature range of 65–70 °C by recovering heat from high-temperature exhaust air (84 °C inlet, 36,000m³/h flow rate). The methodology integrates fundamental thermodynamic assessment (LMTD and ϵ methods) with Computational Fluid Dynamics (CFD) for detailed flow and temperature mapping. Critically, a Differential Evolution (DE) algorithm was applied to optimize plate geometry, channel size, and profile arrangement, subject to a mass constraint, to maximize heat transfer. Results confirm that the optimized design achieves 18-25% natural gas savings and 27.5% higher efficiency compared to conventional systems. This hybrid approach validates the optimized heat exchanger as a highly sustainable and economically viable solution for industrial thermal management.

Keywords: HAET RECOVERY, THERMAL MANAGEMENT

1. Introduction

Industrial dryers are significant energy consumers within manufacturing facilities due to their reliance on high-volume, high-temperature air. Operations across nonwoven, textile, paper, food, and chemical sectors incur substantial energy costs by utilizing fossil fuels (natural gas) or electricity for air heating. Drying is globally recognized as one of the most energy-intensive industrial processes, typically accounting for 10-20% of total industrial energy use in developed nations, primarily due to the necessity of supplying the latent heat of evaporation [1]. Furthermore, convective dryers often exhibit inherently low thermal efficiencies, sometimes below 50% [2]. Minimizing this energy expenditure is crucial for operational sustainability.

The exhaust air discharged at the end of the drying process typically retains substantial thermal energy, frequently ranging from 70-120 oC. This waste heat represents a potential recovery of 20-30% of the total process energy input [3]. Studies estimate that around 29% of the energy supplied to industrial dryers is often wasted or rejected as heat losses [4]. Historically, this energy is vented, resulting in economic loss and adverse environmental consequences, including elevated CO₂ emissions. Effective heat recovery strategies are therefore vital, offering the potential to reduce the specific energy demand of drying processes by 20-80% [5].

This research focuses on the optimized design and analysis of an air-to-air heat recovery unit to exploit this waste energy. The system targets a process where 36,000 m³/h of 84 oC exhaust air preheats the fresh air supply (inlet temperature 25 oC) to 65-70 oC. This preheating action effectively reduces the thermal load demanded from the main burner, thereby significantly improving the system's thermal efficiency and contributing to the reduction of the carbon footprint.

While extensive studies address the general application of heat exchangers, research specifically targeting the geometric optimization of compact plate designs for high-flow industrial exhaust, coupled with both detailed CFD modeling and advanced evolutionary algorithms like Differential Evolution (DE), remains limited. Existing literature often relies on steady-state analytical solutions or focuses solely on fixed geometries. This paper distinguishes itself by employing a rigorous numerical approach, utilizing the DE algorithm to systematically optimize multiple geometric parameters of a high-capacity counter-flow heat exchanger, ensuring both thermal performance maximization and compliance with critical physical constraints (e.g., mass and pressure drop limits).

This paper details the combined theoretical, numerical (CFD), and evolutionary optimization approach used to develop this high-performance heat recovery system.

2. Methodology

2.1. System Configuration and Design Parameters

The heat recovery unit utilizes a compact plate heat exchanger configuration. It is constructed from 399 AISI 316 stainless steel profiles measuring 40×40×2 mm. A counter-flow arrangement is employed, where exhaust air flows externally over the profiles, and fresh air flows internally through the rectangular channels. This configuration inherently maximizes the Log Mean Temperature Difference (LMTD) for enhanced energy transfer. The design and operating parameters are summarized in Table 1:

Table 1: The design and operating parameters		
Parameter	Exhaust Air (Hot Side)	Fresh Air (Cold Side)
Inlet Temperature	84°C	25°C
Outlet Temperature	75–76°C	65–70°C (Target)
Flow Rate	36,000 m ³ /h	18,000 m ³ /h
Pressure Drop	300–400 Pa	300–1000 Pa

The heat exchanger casing incorporates a 1.5° sloped bottom surface to facilitate gravity-assisted drainage of any condensation.

2.2. Thermodynamic Modeling (LMTD and Energy Transfer)

The LMTD method was used to calculate the average temperature difference (ΔT_{lm}) driving the heat transfer (Q).

The LMTD calculation based on design temperatures is:

$$LMTD = \ln(\Delta T_2 \Delta T_1) / (\Delta T_1 - \Delta T_2)$$

For the counter-flow design:

- $\Delta T_1 = T_{h,in} - T_{c,out} = 84^\circ\text{C} - 70^\circ\text{C} = 14^\circ\text{C}$
- $\Delta T_2 = T_{h,out} - T_{c,in} = 75^\circ\text{C} - 25^\circ\text{C} = 50^\circ\text{C}$

The resulting LMTD is approximately 29.2°C.

The total theoretical heat transfer (Q) is calculated using the energy balance for the cold fluid (fresh air):

$$Q=m \cdot c_p \cdot \Delta T$$

With a mass flow rate ($\dot{m}$) of approximately 5.8 kg/s (derived from the 18,000 m³/h flow rate at standard air density) and a target ΔT of 45°C, the theoretical heat transfer is $Q_{\text{theoretical}} \approx 262.2$ kW. Actual field measurements and optimized analysis target a recovered heat range of 120–135 kW.

3. CFD and Optimization

CFD analysis was performed according to the technical specifications of the resulting heat exchanger, and analysis data was obtained. Analysis attempts were made with different profile lengths, layout combinations, and profile offsets. These simulations were used to understand the flow and temperature distribution of the baseline heat exchanger geometry and to create an initial data set for the optimization process.

A Python code utilizing the Differential Evolution (DE) algorithm was developed to optimize the output of a mathematical model created based on specific physical parameters (x: number of vertical profiles, y: number of horizontal profiles, p: profile offset, L: profile length, and D: profile diameter); to best fit this model to the CFD (Computational Fluid Dynamics) results; and simultaneously to determine the optimum geometric and physical parameters that maximize heat transfer, while not exceeding a specific mass limit (approximately 1142 kg). The regression analysis data is presented in Table 1.

Table 1: The regression analysis data

	1S1	1S2	1S3	2S2	P2S3	P3S2	P3S3	P4S2	P4S3	P5S2	P5S3
Horizontal Profile Count (units)		0	4		6	6	6	6	6	6	6
Vertical Profile Count (units)					8	4	4	4	4	4	4
Profile Offset (mm)	0	0	0	0	20	30	40	20	20	20	20
Profile Length (m)					1	1	1	1.5	2	1	1
Circle Diameter (mm)	0	0	0	0	40	40	40	40	40	50	60
Q Heat Transfer Amounts (W)	161	875	430	340	8600	3946	3829	5919	7596	3907	3805

Regression analysis was performed using the analysis data in the table 1, and the following code was structured based on the results of this analysis.

```
Python
import numpy as np
from scipy.optimize import differential_evolution

# Constants
b = 1.5 # mm
rho = 7990 # kg/m^3

# Mass calculation function
def mass(x, y, L, D):
    x = int(round(x))
    y = int(round(y))
    A = (D * b - b**2) * 1e-6 # mm^2 → m^2
    V = 4 * np.pi * x * y * L * A # m^3
    return rho * V # kg

# Q function
def Q_total(x, y, p, L, D):
```

```
    x = int(round(x))
    y = int(round(y))
    q_x = -4.9688 * x**2 + 758 * x - 208.125
    q_y = 10.125 * y**2 + 988.25 * y + 46
    q_p = 0.49 * p**2 - 46 * p + 4885
    q_L = -202 * L**2 + 4041 * L + 322
    q_D = 0.76 * D**2 - 93.8 * D + 6697
    return q_x + q_y + q_p + q_L + q_D

# Objective function
def objective(vars):
    x, y, p, L, D = vars
    x = int(round(x))
    y = int(round(y))
    m = mass(x, y, L, D)
    penalty = abs(m - 1142) * 1000
    return -Q_total(x, y, p, L, D) + penalty

# Variable bounds
bounds = [
    (2, 10), # x (integer)
    (2, 70), # y (integer)
    (20, 30), # p (mm)
    (1, 1.5), # L (m)
    (30, 40) # D (mm)
]

# Optimization
result = differential_evolution(
    objective,
    bounds,
    strategy='best1bin',
    maxiter=1000,
    tol=1e-6,
    seed=42
)

# Results
x_opt, y_opt, p_opt, L_opt, D_opt = result.x
x_opt = int(round(x_opt))
y_opt = int(round(y_opt))

m_opt = mass(x_opt, y_opt, L_opt, D_opt)
Q_opt = Q_total(x_opt, y_opt, p_opt, L_opt, D_opt)

# Print
print("\n--- OPTIMAL VALUES (x, y integer) ---")
print(f"x = {x_opt}")
print(f"y = {y_opt}")
print(f"p = {p_opt:.2f} mm")
print(f"L = {L_opt:.2f} m")
print(f"D = {D_opt:.2f} mm")
print(f"Q (heat transfer) = {Q_opt:.2f} W")
print(f"m (mass) = {m_opt:.2f} kg")
```

Key Results Obtained from CFD Analysis are shown in Table 2.

Table 2: Key Results Obtained from CFD Analysis

Parameter	Value
Fresh Air Outlet Temperature	313.57 K(≈40.4°C)
Total Heat Transfer Rate	-120,412.22 W
Exhaust Air Outlet Temperature	341.98 K(≈68.9°C)
Fresh Air Pressure Drop	1003.25 Pa
Exhaust Air Pressure Drop	377.89 Pa

The initial 40.4°C outlet temperature shows that the baseline design did not meet the 65–70°C target. This outcome highlighted the necessity for systematic optimization, providing the empirical foundation for the subsequent optimization phase. The reported Heat Transfer Rate (120.4 kW) represents the recovered energy in the unoptimized state.

3.2. Geometric Optimization via Differential Evolution (DE)

The low $T_{c,out}$ of 40.4 °C relative to the design target necessitated a systematic optimization of the heat exchanger geometry. The optimization problem was formulated to maximize the total

recovered heat (Q) while strictly adhering to dimensional and mass constraints, thereby minimizing the parasitic energy consumption (fan power) associated with high pressure drops [11].

The Differential Evolution (DE) algorithm [12] was employed to iteratively solve this constrained maximization problem. DE is a robust, population-based search technique well-suited for non-linear, multi-dimensional objective functions encountered in thermal system design.

The optimization problem is defined as:

Maximize $Q(X)$ Subject to constraints

Where X is the vector of geometric design variables:

$X = \{x, y, p, L, D\}$

(where x and y are integer-constrained profile counts, p is the offset, L is the length, and D is the profile diameter).

Objective Function and Constraints

The objective function $f(X)$ was designed to maximize the heat transfer rate Q while penalizing solutions that violated the mass limit (M_{max}):

Objective Function = Minimize $[-Q(X) + C \cdot \max(0, M(X) - M_{max})]$

Where:

$Q(X)$: The heat transfer rate (derived empirically from CFD data).

$M(X)$: The mass of the heat exchanger, calculated as a function of the geometric variables X .

M_{max} approx 1142 kg: The maximum allowable mass constraint.

C : A large penalty constant to enforce the mass constraint [13].

The geometric boundaries for the DE search space were defined to ensure physical feasibility and are crucial for the algorithm's convergence efficiency. The constraints primarily focused on the maximum allowable mass and the maximum allowable pressure drop (ΔP_{max}) across the fresh air circuit, as this dictates the size and power of the industrial fan [11].

The successful convergence of the DE algorithm identified the optimal combination of profile counts (x, y) and dimensions (p, L, D). This ensured the final heat exchanger geometry achieved the thermal target ($T_{c,out} = 65-70$ oC) while balancing the trade-off between heat transfer maximization and hydraulic performance (i.e., maintaining ΔP within acceptable limits). The resulting design represents a techno-economically optimal solution for industrial integration [13].

Graphical values for the designed heat exchanger are given in Figures 1-5, the Temperature Gradient is given in Figure 6, and the Inlets and Outlets of the Designed Heat Exchanger are given in Figure 7.

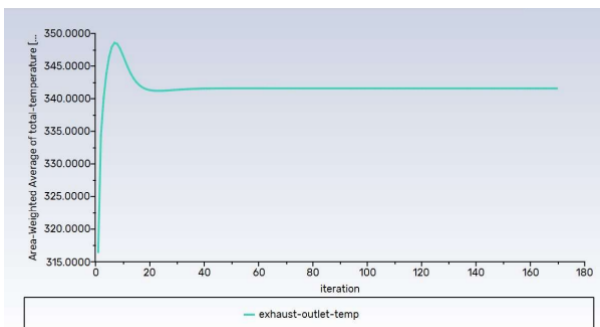


Figure 1. Exhaust Temperature Profile at the Outlet

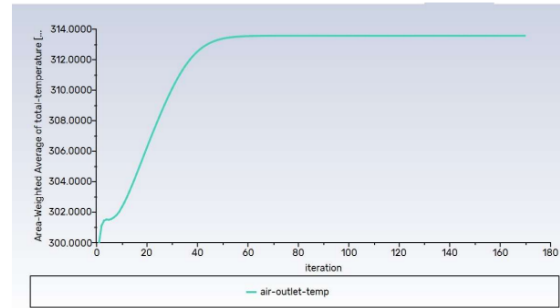


Figure 2. Fresh Air Temperature Profile at the Outlet

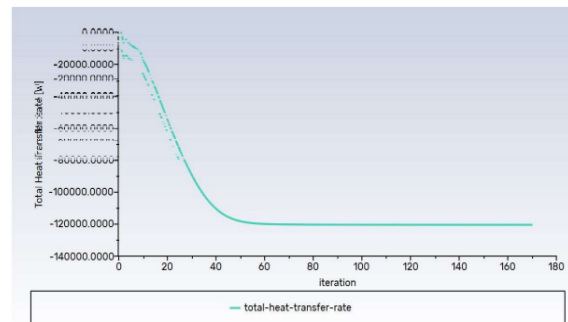


Figure 3. Total Heat Transfer

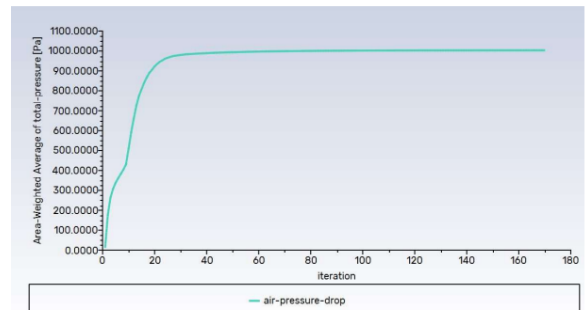


Figure 4. Fresh Air Pressure Drop

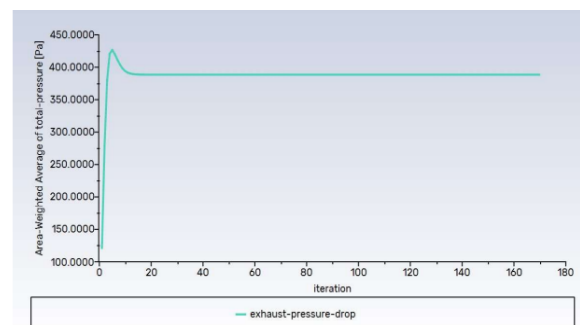


Figure 5. Exhaust Pressure Drop

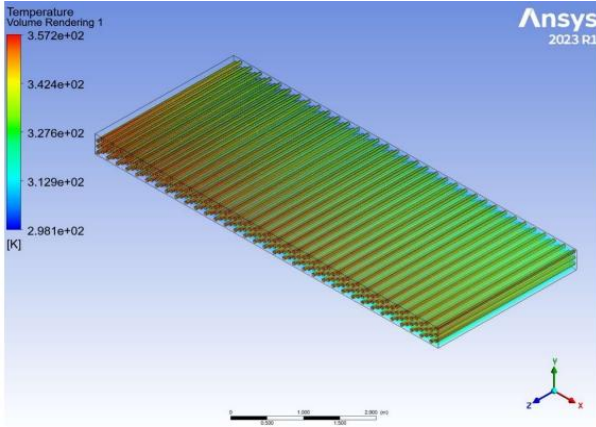


Figure 6. Temperature Gradient

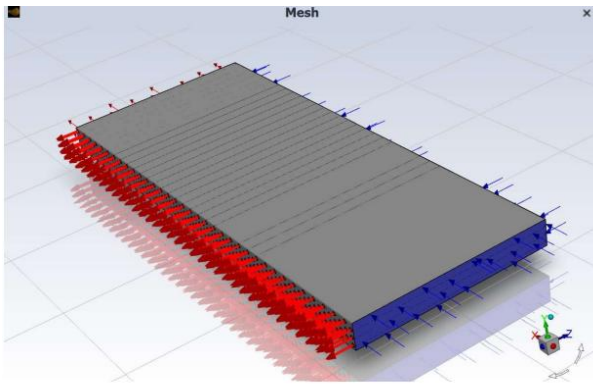


Figure 7. Inlets and Outlets of the Designed Heat Exchanger

4. Results and Economic Impact

The implementation of the optimized air-to-air heat recovery system results in significant energy savings and operational cost reductions.

1. Thermal Energy Savings:

The system provides a steady preheating capacity that corresponds to a 18-25% reduction in annual natural gas consumption. Furthermore, analysis shows that the optimized heat exchanger exhibits an efficiency improvement of 27.5% over older, non-optimized systems commonly used in the industry, highlighting the significant impact of the design methodology.

2. Economic Impact:

The substantial decrease in fuel consumption translates into annual energy cost savings estimated between 3000 – 6000 €. Such rapid return on investment (ROI) is crucial for justifying the capital expenditure associated with the heat recovery unit [15].

3. Environmental Benefits:

The reduction in natural gas combustion directly leads to a 10-20% decrease in annual CO₂ emissions, significantly improving the environmental profile of the industrial operation and aligning the facility with sustainability goals [16].

The synthesized results confirm that the designed waste heat recovery system is an KANSAN innovative engineering solution that simultaneously addresses three key industrial concerns: energy cost reduction, process stability enhancement, and environmental mitigation.

5. References

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FEA-Driven Design of Nonwoven Winder Drums: Stress Minimization and Rigidity Assessment for Structural Integrity

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Abstract: Nonwoven winding machines are critical equipment where the structural integrity of the main drum directly impacts the quality and stability of the final product. This study presents the mechanical analysis and braking system design for a main winding drum (Diameter 400 mm) in a high-speed nonwoven application, driven by Finite Element Analysis (FEA) for stress minimization. The load analysis, based on the Principles of Static Equilibrium, determined the total maximum load on the drum supports, considering a maximum spool weight of 1500 kg and a nip force of 1962 N. The resultant total load applied on the supports was calculated as approximately 11.5 kN. The FEA, utilizing ST37 steel, revealed a maximum Von Mises Stress of 1.754 MPa and an extremely low maximum deflection of 0.005 mm. This confirms an optimal factor of safety (FS approx 134) and high rigidity. Furthermore, the paper addresses the safety requirement for emergency stopping from a maximum speed ($\omega = 50$ rad/s). The minimum required braking torque was calculated as 235 Nm, while the selected COREMO PNEUMATIC CALIPER BRAKE B-2N system provides 306.8 Nm, ensuring reliable and controlled deceleration. The results validate the structural and functional design, contributing to enhanced machine performance and operational safety.

Keywords: FEA-DRIVEN DESIGN, STRESS MINIMIZATION, STRUCTURAL RIGIDITY, WINDING DYNAMICS

1. Introduction

Nonwoven winding machines are central to the production chain in industries ranging from hygiene and medical textiles to automotive and geotextiles, where wide nonwoven webs must be accurately slit and rewound into stable, high-quality finished rolls (reels) [1].

The efficiency and quality of the final product depend critically on the control of the web handling process, particularly the precision applied to Tension, Nip, and Torque (TNT) parameters throughout the winding cycle [2, 3]. Failure to maintain optimum control can lead to costly defects such as telescoping, starring, wrinkling, buckling, and layer slippage, which compromise product performance and structural integrity [4, 5].

Structural and Dynamic Challenges of Winder Drums

The main drum (winding roller) serves as the primary load-bearing and driving element in most surface or two-drum winding configurations [6]. Its design is subjected to complex static and dynamic loading conditions.

The primary structural challenge lies in managing the combined loads from the increasing weight of the final spool (which can exceed 1500 kg), the controlled pressure exerted by the rider roll (nip force), and the continuous web tension [7].

High-speed operation introduces significant rotordynamic effects. As the rotational speed of the roll intersects with the natural frequencies of the winder system, resonance can occur, leading to phenomena like roll bouncing and excessive machine vibration [8, 9]. Previous research emphasizes that winder design must be guided by the principle that major excitation sources, such as manufacturing imperfections or polygonization of viscoelastic components, should not coincide with the system's resonance frequencies [10, 11]. Therefore, a comprehensive Finite Element Analysis (FEA) is necessary to evaluate the structural stress distribution and confirm that the drum's rigidity is sufficient to prevent critical deflection and guarantee stable operation [12].

The Critical Role of Braking and Inertia Control

Maintaining constant web tension and ensuring operational safety relies heavily on the deceleration mechanism. The braking system is vital not only for precise tension control during normal operation but also for emergency stopping. High-speed winders, operating at speeds up to 600 m/min, possess high rotational inertia [16]. A safe, rapid, and controlled deceleration requires a braking system (such as highly reliable pneumatic caliper brakes) capable of delivering a high torque output to absorb the total kinetic energy of the rotating masses within a very short timeframe [17]. The thermal energy generated during this process must also be managed to prevent brake performance degradation [18].

This study focuses on providing a validated engineering solution for the main drum structure and its associated deceleration mechanism, utilizing FEA as the primary verification tool. We first conduct a detailed Static Equilibrium analysis to accurately model the complex loading profile on the Diameter 400 mm main drum. Subsequently, we utilize FEA to confirm stress minimization, high factor of safety, and minimal deflection under maximum operating conditions. Finally, we design and size a specific Pnömatic Caliper Brake system to meet the critical emergency stopping requirements dictated by the system's high inertia and speed.

2. Theoretical Background and Methodology

The Schematic Representation and Free-Body Diagram of the Main Drum are given in Figure 1 and Figure 2, respectively

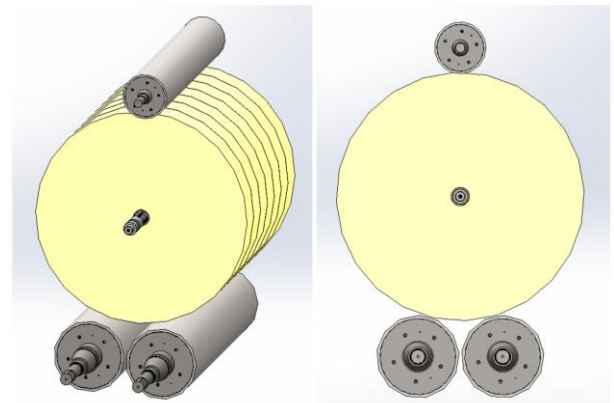


Figure 1. Schematic Representation of the Main Drum

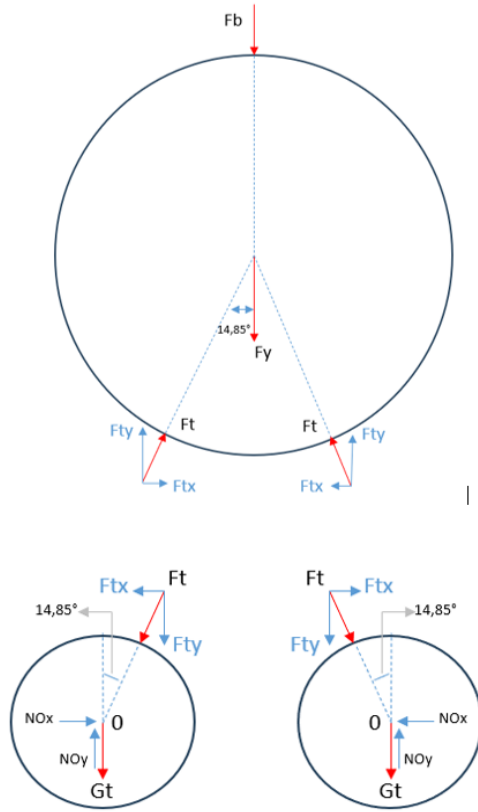


Figure 2. Free-Body Diagram of the Main Drum

2.1. Load Analysis based on Static Equilibrium

The main drum's static loads were calculated based on the Principles of Static Equilibrium ($\Sigma F_y = 0$). The drum material is ST37 structural steel. The primary vertical loads are given in Table 1. (assuming $g=9.81 \text{ m/s}^2$)

Table 1. The primary vertical loads

Load Component	kg	N
Spool Load Force (F_y)	1500	14715
Nip / Pressure Force (F_b)	200	1962
Drum Weight (G_t)	566	5552,46
Total Bearing Reaction Force (per Support) (F_t)	1172	11498
Vertical Component (per Support) (F_{ty})	1132	11107
Horizontal Component (per Support) (F_{tx})	300	2942

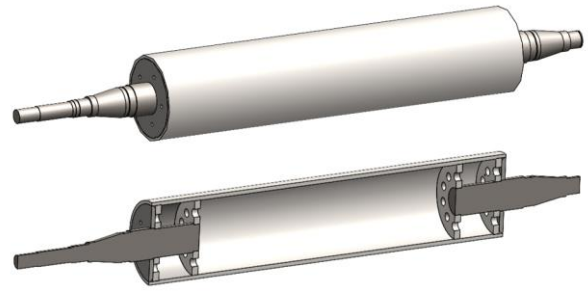
The total downward load is balanced by the two bearing reaction forces (F_t). Assuming the bearing reaction acts at an angle $\theta = 15^\circ$ from the vertical:

$$\text{Total Downward Load} = 22229.46 \text{ N}$$

The resultant force (F_t) on each bearing is:

$$F_t = (F_y + F_b + G_t) / 2 \cos(15) = 22229.46 / 2 \times 0.966 = \text{approx } 11498 \text{ N}$$

A conservative load of 12,000 N (12 kN) was used for the FEA simulation to ensure an additional safety margin.



Main Drum Sectional View

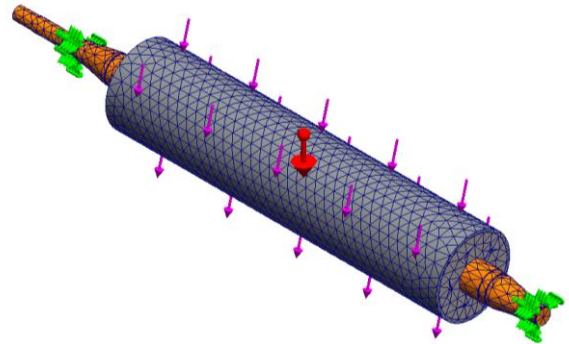


Figure 3. Main Drum Meshing Configuration

2.2. Finite Element Analysis (FEA)

Static structural analyses were carried out using SolidWorks Simulation (CosmosWorks). The objective of the FEA was to verify that the drum design minimized internal stresses and maintained high rigidity under the defined operational loads, thereby validating the design for structural integrity.

3. Structural Analysis Results and Discussion

3.1. Maximum Stress (Von Mises) Analysis

The FEA results confirmed the structural integrity of the drum:

Maximum Von Mises Stress ($\sigma_{\max}$): 1.754 MPa

Material Yield Strength (σ_y): 235 MPa (ST37 steel)

The resultant Factor of Safety (FS) is calculated as:

$$FS = (\sigma_y) / (\sigma_{\max}) = 235 \text{ MPa} / 1.754 \text{ MPa} = \text{approx } 134$$

The exceptionally high safety factor demonstrates that the FEA-driven design has successfully minimized stress concentrations, guaranteeing high structural integrity and reliability.

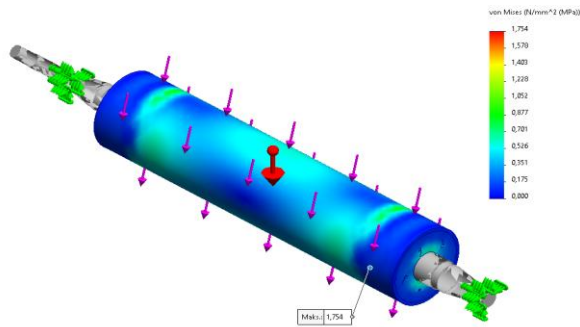


Figure 4. Stress Distribution Analysis of the Main Drum

3.2. Maximum Displacement (Rigidity Assessment)

Maintaining minimal displacement is crucial for winding quality.

Maximum Deflection (δ_{max}): 0.005 mm

This remarkably low displacement value confirms the drum's high stiffness. The rigidity assessment proves that the chosen geometry and ST37 material combination ensures that the drum maintains its precise surface profile, preventing dimensional errors and quality degradation during high-speed winding.

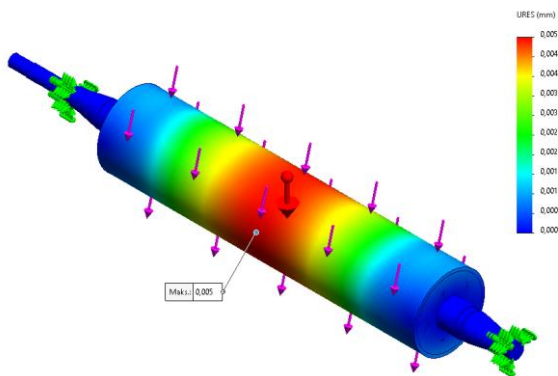


Figure 5. Analysis of Max. Displacement in the Main Drum

4. Braking System Design and Deceleration Control

A Pnömatic Caliper Brake system was selected to manage the high kinetic energy of the system during emergency stops and controlled deceleration.

4.1. Required Braking Torque Calculation

The braking system must ensure a safe stop within $t=3$ s from the maximum angular velocity ($\omega = 50$ rad/s).

- Drum Inertia (J_{drum}): 14.10 kg m²

The minimum required torque ($T_{required}$) is:

$$T_{required} = J_{drum} \cdot \omega / t$$

$$T_{required} = 14.10 \cdot 50 / 3 = \text{approx } 235 \text{ Nm}$$

4.2. Selected Brake System and Torque Capacity

The selected system is the Coremo Pneumatic Caliper Brake (Negative-Acting B-2N) with an A1303 brake disc.

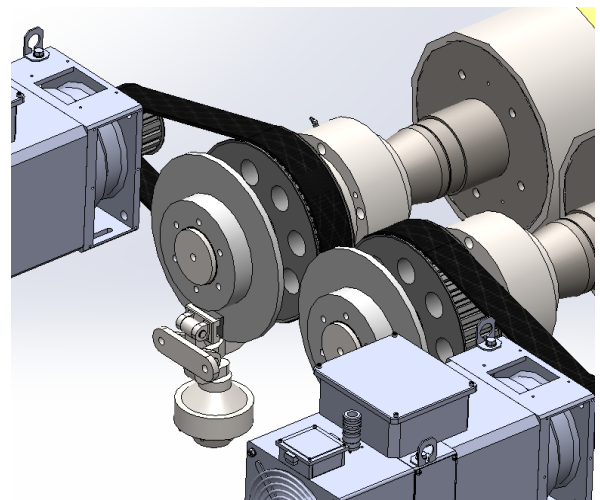


Figure 6. Pneumatic Caliper Brake

- Braking Force (F): 2600 N

The actual braking torque (T_{brake}) provided is:

$$T_{brake} = 2600 \text{ N} (0.15 \text{ m} - 0.032 \text{ m}) = 306.8 \text{ Nm}$$

4.3. Safety Margin Assessment

The provided braking torque of 306.8 Nm significantly exceeds the minimum required torque of 235 Nm. This margin ensures the system's robust performance in safety-critical situations, accounting for operational variations and friction losses.

Numerical analysis of substrate influence on fracture mechanisms in PVD deposited TiN coatings

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Abstract: Coatings of titanium nitride (TiN) are widely used due to their high hardness and wear resistance, making them suitable for protective, decorative, and semiconductor applications. However, their tendency toward brittle cracking and low fracture toughness limits their performance in demanding environments. Understanding and accurately modelling fracture behaviour in TiN is therefore essential to improving reliability in microelectronics, protective coatings, or biomedical devices. This work presents a first approach to modelling fractures in TiN films by explicitly representing their columnar morphology. A procedure for generating statistically representative digital microstructures and incorporating them into finite element simulations is described. The approach uses a hybrid cohesive–XFEM fracture model to capture crack initiation and propagation under complex deformation states, particularly during nanoindentation. The numerical results are validated with results from a scanning electron microscopy (SEM) investigation.

KEYWORDS: COATINGS, CZM, XFEM, FRACTURE MECHANISMS, OPENCV

1. Introduction

Nowadays, there is a growing demand for new methods to extend the functionality of devices used across key industrial areas. Therefore, composites comprising multiple thin films of conventional materials are increasingly used to improve the properties of the final product. One of the most popular techniques for creating these composites is the PVD (Physical Vapor Deposition) method. It consists of the material's target evaporation and its synthesis with the substrate, characterized by nanoscale accuracy in the creation of thin films and coatings [1]. Another technique used in this work is the PLD (Pulsed Laser Deposition), schematically shown in Fig. 1a. This method is based on laser ablation, which involves local evaporation of the target material using a laser beam. The plasma containing the material atoms is then transported to the substrate, where it condenses to form the thin film structure (Fig. 1b).

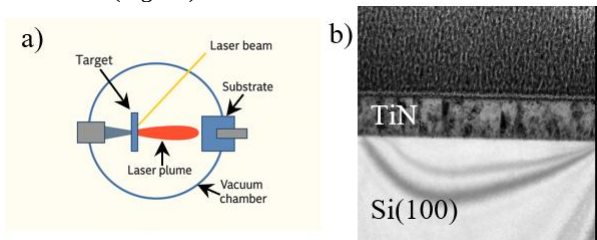


Fig. 1. a) Concept of PLD, b) TEM image of TiN film on Si(100) substrate.

2. Thin films morphology

Since the deposition process involves transporting plasma onto the substrate, the resulting morphology often depends on the chamber's operating parameters. Thornton's model has extensively described the possible film morphologies. This model is one of the basic diagrams illustrating the possible growth of the polycrystalline microstructure of thin films deposited physically from the gas phase [2]. The growth of the columns is represented as a map with four distinct zones, each corresponding to different column density and composition characteristics as shown on Fig. 2. The horizontal axis represents the ratio between the substrate temperature and the melting temperature of the deposited material.

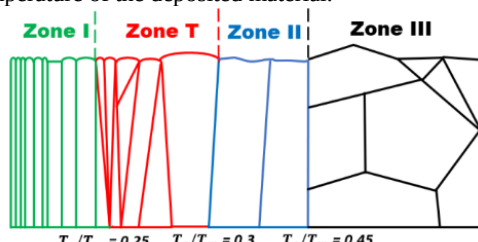


Fig. 2 Schematical illustration of Thornton's model.

Film behaviour under loading conditions is often evaluated using the nanoindentation technique. Since it probes extremely small volumes, nanoindentation is especially valuable for thin films and coatings where conventional mechanical testing is not feasible.

3. Numerical model of the nanoindentation test

As mentioned, nanoindentation is used to analyse the mechanical properties of films and coatings. It involves inserting a diamond tip of a specific shape into the material's surface while simultaneously monitoring the applied force and the corresponding displacement. From this data, information on the material's mechanical response can be extracted [3].

In this work, a numerical model for this test was created using a plug-in implemented in Abaqus CAE software, which automated the process of creating models ready for nanoindentation analyses. Based on this plug-in, a 2D planar model was created, including:

- Conical indenter with a spherical tip with a radius of 1 μm , which was considered as an analytical rigid shell.
- Thin film 0.1 μm thick and 15 μm wide, consisting of 100 funnel-shaped columns representing film morphology, defined as a deformable shell.
- Substrate of the selected material, defined as a deformable shell with dimensions of 30 $\times$ 50 μm .

Additionally, the concentrated force was applied to the indenter, with a value of 1 gf (0.0098 N). Fig. 3 illustrates the developed 2D model used to conduct numerical simulations of the nanoindentation process.

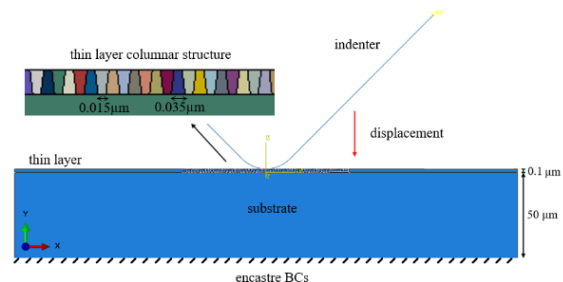


Fig. 3. 2D Numerical model of the nanoindentation process.

The aim of this work was to determine the crack characteristics of the Titanium Nitride (TiN) thin film deposited on 2 different material hardness bases: stainless steel (SS316L) and aluminum (Al 1050). Material data were derived from literature[4, 5]. A simplified rheological model of Swift-type hardening was used (1) $\sigma = (A + B \cdot \epsilon^n)$.

$$(1) \quad \sigma = (A + B \cdot \epsilon^n)$$

where: σ – yield stress, A – initial yield strength, B – strain hardening constant, ϵ – plastic strain, n – strain hardening exponent.

In the presented model, two numerical methods were used to model fracture mechanisms: the cohesion zone method (CZM) and the extended finite element method (XFEM). The CZM method is based on a traction-separation law that represents the fracture mechanism at the boundary of TiN microstructure columns (Fig. 4a) and at the delamination between the thin film and the substrate (Fig.

4b). The XFEM model depends on the maximum nominal stress at the crack tip and can predict fractures within the columns (Fig. 4c).

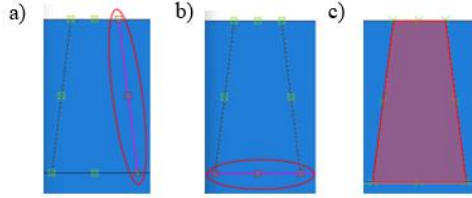


Fig. 4. Assignment of the CZM to a) intercolumn boundary, b) column-substrate boundary and XFEM to c) intracolumn area.

These models assume initial linear-elastic behaviour, followed by crack formation and propagation. To simulate fracture development, it is necessary to define a crack initialization and propagation criteria, in which the maximum nominal stresses (σ_{max}) and total displacement (δ_c) can be specified. These parameters were analytically determined using the critical stress-intensity K_{IC} factor calculated according to the formula (2) $K_{IC} = \sqrt{\frac{1}{2} \sigma_{max} \delta_c E}$ [4]. Values for crack initialization and propagation are listed in Table 1.

$$(2) \quad K_{IC} = \sqrt{\frac{1}{2} \sigma_{max} \delta_c E}$$

where: E – Young modulus, σ_{max} – maximal nominal stress, δ_c – total displacement.

Table 1. Fracture parameters for crack nucleation and growth for CZM (intercolumn, delamination) and XFEM (intracolumn).

	CZM		XFEM
criterion	intercolumn	delamination	intracolumn
σ_{max} [GPa]	5	10	5.5
δ_c [μ m]	1E-05	1E-05	1E-05

4. Simulation results

Numerical simulations were conducted using a hybrid (CZM, XFEM) method, which resulted in the formation of numerous cracks in thin TiN films on all base materials. Fig. 5 presents the result of combining both CZM and XFEM methods, where all three fracture mechanisms: intercolumnar, intracolumnar, and delamination are simultaneously visible.

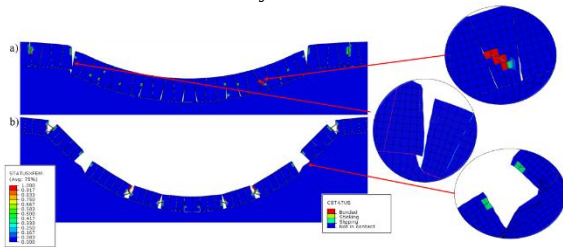


Fig. 5 Hybrid CZM and XFEM fracture model of a thin TiN film on a) SS316L and b) Al 1050.

The OpenCV library was used to develop a script that automates the verification of the dimensions of structures formed in a thin TiN film deposited on an Al1050 substrate after the nanoindentation simulation as presented in Fig. 6.

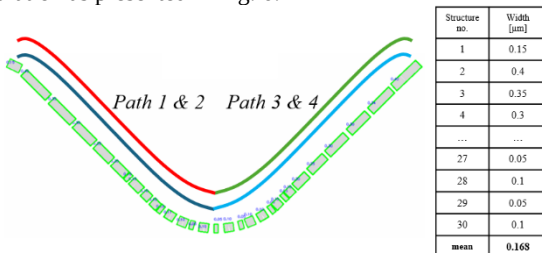


Fig. 6 Calculated widths of the structures after numerical simulation.

The average structure sizes in individual simulations were then compared with the average structure sizes obtained from 4 different paths, determined from SEM imaging of the sample surface after nanoindentation, as shown in Fig. 7.

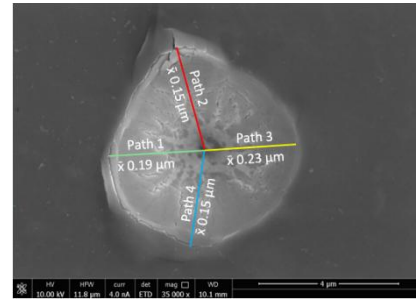


Fig. 7 Average TiN-Al 1050 structure sizes of 4 paths from [3].

Table 2 shows the accuracy of the simulation results compared to the laboratory results, calculated as the relative error.

Table 2. Calculated relative error of the mean structure sizes.

	Simulation 1	Simulation 2	Simulation 3	Simulation 4
Path 1	88.13%	96.86%	89.75%	69.72%
Path 2	87.78%	76.67%	85.71%	88.77%
Path 3	88.52%	77.48%	86.47%	88.18%
Path 4	71.94%	79.06%	73.26%	56.91%

5. Conclusion

The aim of this work was to demonstrate the potential of finite element method calculations in conjunction with OpenCV image analysis techniques to predict fracture in thin films.

The key factor enabling the observation of cracking was the development of a model representing the columnar morphological structure of a thin TiN film, in which cracks were modelled using CZM and XFEM methods.

The presented numerical method can be widely used in the virtual testing of thin films. Numerical simulations enable the prediction of the impact of various parameters, such as the thickness of deposited films, the properties of the base material, or the film's morphology, saving time and resources that would otherwise be required to conduct a series of costly laboratory experiments.

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Comparative study of different kinetic models for lactic acid production

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Abstract: This study set out to model lactic acid production from lactose and dilute-acid DDGS hydrolysates used as substrates by *Lactiplantibacillus plantarum* AC 11S, and to identify the mathematical model that best represents the experimental data. An unstructured model was formulated, incorporating equations for microbial growth, substrate utilization, and product formation. The model was evaluated using different expressions for the specific growth rate, including cases with substrate and/or product inhibition. Parameter values for the various model versions were estimated and compared. When only the biomass-growth equation was solved for different initial substrate concentrations, the modified Gompertz model provided the best fit. However, when the full system of differential equations was applied, a logistic-type growth expression yielded the most accurate results. Simulations at different initial biomass levels indicated that higher biomass shortened the lag phase and enabled the culture to reach stationary phase more quickly. A key benefit of well-constructed fermentation models is their capacity to predict system behavior under varying conditions. Using the obtained parameter estimates, additional calculations were carried out to forecast how initial biomass concentration affects process performance.

KEYWORDS: LACTIC ACID PRODUCTION; *LACTIPLANTIBACILLUS PLANTARUM*; LACTOSE; DISTILLERS DRIED GRAINS; PH-CONTROLLED FERMENTATION; PROCESS MODELING

1. Introduction

Lactic acid bacteria (LAB) comprise a broad and diverse group of microorganisms recognized for their important contributions to food processing and pharmaceutical fields. While LAB strains share general metabolic and physiological features, each strain possesses distinct functional properties. Their hallmark trait is the ability to ferment a wide range of carbohydrates into lactic acid.

From a taxonomic viewpoint, LAB include numerous Gram-positive, catalase-negative, non-spore-forming anaerobes within the *Lactobacillaceae* family, distributed across several Firmicutes groups with varying G+C contents. These bacteria produce a variety of metabolites, such as organic acids, polyols, bacteriocins, exopolysaccharides (EPSs), and aromatic compounds [1]. Moreover, many LAB species are recognized as probiotics, offering functional attributes and health-promoting effects linked to their metabolic activity.

Lactiplantibacillus plantarum inhabits a wide range of ecological environments, including dairy products, fermented vegetables and grains, meat, fish, silage, wine, and the gastrointestinal, urogenital, and vaginal tracts [2]. It is among the most extensively used LAB for the production of diverse postmetabolites and is well recognized for its broad substrate-utilization capabilities [3].

This species is classified as a facultatively heterofermentative lactobacillus. Through the Embden–Meyerhof–Parnas pathway, it converts hexose sugars almost entirely into lactic acid, whereas pentoses are transformed into both acetic and lactic acids via the 6-phosphogluconate/phosphoketolase pathway, activated by phosphoketolase induction [4]. Like other LAB, *L. plantarum* requires specific nutrients and thus thrives in complex media containing peptides, vitamins, nucleic and fatty acids, amino acids, and an appropriate carbon source.

A key challenge in lactic acid fermentation is end-product inhibition: as lactic acid accumulates, rapid acidification of the medium occurs, which subsequently reduces substrate consumption, conversion efficiency, and the final concentration of the product.

Kinetic analysis is an essential component of any thorough investigation into lactic acid production. A well-constructed mathematical model is invaluable for understanding, describing, assessing, and predicting fermentation behavior. Such models clarify the relationships among microbial growth, substrate depletion, and product formation, and they serve as important tools for process control, optimization, and scale-up. Various criteria have been used to classify mathematical models [5]. One common distinction is between structured and unstructured models. Structured models offer higher accuracy by accounting for cellular composition, structure, and metabolic functions, while unstructured models treat cells as a single entity without considering physiological details. Although structured models provide deeper insight into system behavior, unstructured models are widely applied because they are simpler and still effective for describing microbial kinetics.

Numerous modeling approaches have been employed to describe lactic acid fermentation from different substrates, with several summarized in the works of Zacharof & Lovitt [5], Bouguettoucha et al. [6], and Gordeev et al. [7].

The goal of the present study is to evaluate and compare several kinetic models that describe the fermentation process of lactic acid production from lactose and DDGS hydrolysates by *Lactiplantibacillus plantarum* AC 11S.

2. Materials and Methods

2.1. Strain, Growth Media, and Culture Conditions

L. plantarum AC 11S was originally isolated from homemade white brined cheese [8]. The strain was maintained in de Man, Rogosa, and Sharpe (MRS) broth (Merck, Darmstadt, Germany) and stored at -20°C in MRS supplemented with 20% (v/v) glycerol. Prior to experimentation, it was subcultured twice in a lactose-modified MRS medium.

For cultivation, the strain was grown in a medium containing 11 g/L lactose monohydrate, 5.5 g/L yeast extract, 12.5 g/L casein peptone, 10 g/L sodium acetate, 0.25 g/L KH_2PO_4 , 0.25 g/L K_2HPO_4 , 0.1 g/L $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$, 0.05 g/L $\text{MnSO}_4 \cdot 7\text{H}_2\text{O}$, and 0.05 g/L $\text{Fe}_2(\text{SO}_4)_3$. All reagents were analytical grade (Fluka, Darmstadt, Germany). The inoculum (10% v/v) was prepared from an overnight culture in MRS medium containing 11 g/L lactose monohydrate.

Experiments were performed in 300-mL Erlenmeyer flasks with 100 mL of growth medium, incubated at 30°C and an initial pH of 6.5, using a WiseCube® WIS30 shaking incubator (Witeg Labortechnik GmbH, Wertheim, Germany).

2.2. Lactose and DDGS hydrolysates fermentation

An MRS medium was prepared with the following composition (g/L): yeast extract 5.5, peptone 12.5, KH_2PO_4 0.25, K_2HPO_4 0.25, sodium acetate 10.0, $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$ 0.1, $\text{MnSO}_4 \cdot 4\text{H}_2\text{O}$ 0.05, $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$ 0.05, and distilled water up to 1000 mL, adjusted to pH 6.5.

Four experimental series were conducted using *L. plantarum* AC 11S with lactose or DDGS hydrolysates as substrates, both with and without pH control, at 30°C .

In the first series, lactose was supplied at three concentrations: 10, 20, and 30 g/L. In the second series, DDGS hydrolysates containing 10, 20, and 30 g/L of reducing sugars were used. Lactic acid fermentations without pH regulation were carried out in 300-mL Erlenmeyer flasks containing 100 mL of medium. Experiments with controlled pH were performed in a BioFlo fermentor (New Brunswick Scientific, Edison, NJ, USA) with a 300-mL working volume under static conditions at 30°C .

Reducing sugars used as substrates were produced through sequential dilute-acid and enzymatic hydrolysis of DDGS. First, 500 mL of a 20% (w/v) dry-matter suspension was subjected to hydrolysis in an autoclave using 1% H_2SO_4 at 2 atm for 1 hour. The acid hydrolysate was then treated with cellulase “Onozuka R-10”

(Yakult Pharmaceutical Industries Co., Ltd., Japan) at pH 4.6 and 45 °C, using an enzyme loading of 40 U/g of substrate for 24 hours. Portions of the resulting hydrolysate were collected and adjusted to the required reducing sugar concentrations for fermentation. All DDGS pretreatment experiments were performed in triplicate, and the fermentation trials were carried out in duplicate. Each sample was analyzed in triplicate, and the data are reported as mean values $\pm$ standard deviation (SD).

2.3. Modeling

A characteristic challenge in modeling biotechnological processes is the large number of parameters required in the mathematical description. Identifying these parameters can be difficult because the least-squares objective function often has multiple extrema or ravine-type minima. Effective parameter estimation therefore depends on using good initial values located near the global minimum area.

In fermentation processes, the primary objective is complete substrate consumption to achieve the highest possible product yield. Developing an appropriate mathematical model and accurately determining its parameters enable operation of the fermentation under optimal conditions. Such a model should include equations that describe cell growth, substrate utilization, product formation, and the relationships among these variables. In unstructured models, the total biomass concentration is the only cell-related variable considered. Generally, bacterial growth can be expressed as follows:

$$\frac{dX}{dt} = \mu X - k_d X \quad (1)$$

where X is the cell concentration, g/L; t is time; μ is the specific growth rate, h^{-1} and k_d is the specific cell death rate. In many cases, the cell death was not observed and the second term can be omitted. Many authors insert different terms in the Monod equation to take inhibition effects into account.

Table 1. Modified Monod models describing cell growth

No	Model name	Equation of biomass specific growth rate	Ref.
1	Verhulst	$\mu = \mu_{\max} \left(1 - \frac{X}{X_{\max}}\right)^n$ if $n \neq 1$ $\mu = \mu_{\max} \left(1 - \frac{X}{X_{\max}}\right)$	[9]
2	Altioik	$\mu = \mu_{\max} \left(1 - \frac{X}{X_{\max}}\right)^{n_1} \left(1 - \frac{P}{P_{\max}}\right)^{n_2}$ if $n_1, n_2 = 1$ $\mu = \mu_{\max} \left(1 - \frac{X}{X_{\max}}\right) \left(1 - \frac{P}{P_{\max}}\right)$	[10]
3	Aiba	$\mu = \mu_{\max} \left(\frac{S}{k_s + S}\right) e^{-k_p P}$	[11]
4	Andrews	$\mu = \mu_{\max} \left(\frac{S}{k_s + S + S^2 / k_i}\right)$	[12]
5	Akerberg	$\mu = \mu_{\max} \left(\frac{S}{k_s + S + S^2 / k_i}\right) (1 - k_p P)^n$	[13]
6	Monod-Jerusalimsky	$\mu = \mu_{\max} \left(\frac{S}{k_s + S}\right) \left(\frac{k_p}{k_p + P}\right)$	[14]
7	Hinshelwood	$\mu = \mu_{\max} \left(\frac{S}{k_s + S}\right) (1 - k_p P)$	[15]

The simplest model representing the specific growth rate as a function of substrate (lactose) concentration is the Monod equation:

$$\mu = \mu_{\max} \left(\frac{S}{k_s + S}\right) \quad (2)$$

where $\mu_{\max}$ is the maximum specific growth rate, h^{-1} ; S is the initial substrate concentration, g/L; K_s – the substrate saturation constant, g/L. The Monod equation describes the increase of cell concentration with time and considers limiting substrate

concentration. It is widely accepted that lactic acid fermentation is limited by substrate and inhibited by the product.

We used the Verhulst equation to describe the specific growth rate as a function of substrate (DDGS hydrolysates) concentration [9]:

$$\mu = \mu_{\max} \left(1 - \frac{X}{X_{\max}}\right)^n \quad (3)$$

The Luedeking – Piret equation [16] is the most used for the description of lactic acid formation. It takes into account the fact that the rate of product accumulation dP/dt , depends on bacterial growth dX/dt , as well as on the bacterial density X .

$$\frac{dP}{dt} = \alpha \frac{dX}{dt} + \beta X \quad (4)$$

α and β are coefficients related to growth and non-growth product formation.

The rate of substrate consumption is closely related to the cell's growth rate and the rate of product formation. This relationship is usually given by the following equation:

$$\frac{dS}{dt} = -\frac{1}{Y_{X/S}} \frac{dX}{dt} - \frac{1}{Y_{P/S}} \frac{dP}{dt} - m_s X \quad (5)$$

where $Y_{X/S}$ and $Y_{P/S}$ are yield coefficients for biomass on substrate and product on substrate respectively, g/g, while m_s is the biomass maintenance energy coefficient, g/g.h. In many cases, the latter was neglected.

3. Results

3.1. Influence of initial substrate concentration

To examine how substrate concentration affects cell growth and lactic acid formation, a series of experiments was carried-out at 30 °C and an initial pH of 6.5 using lactose monohydrate at 11, 22, 33, 44, and 55 g/L, without pH control throughout fermentation. The results are shown in Figure 1. As evident from the figure, at 11 g/L lactose the substrate was nearly fully converted, reaching values close to the theoretical maximum. However, conversion efficiency declined as the substrate concentration increased, likely due to inhibition caused by high substrate levels and/or lactic acid accumulation. Notably, no cell death was detected over the approximately 50-hour fermentation period.

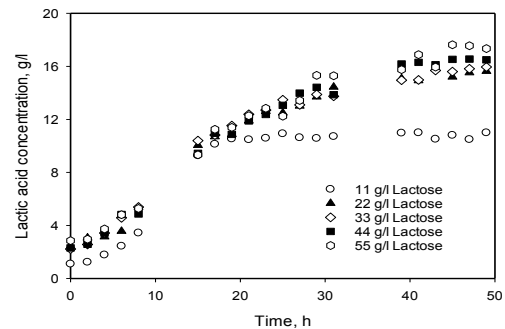


Figure 1. Influence of initial substrate concentration on the lactic acid production at 30 °C and initial pH value 6.5 without pH control.

3.2. Modeling of cell growth, substrate consumption, and product accumulation

The set of differential equations describing the process is:

$$\begin{aligned} \frac{dX}{dt} &= \mu X \\ \frac{dS}{dt} &= -\frac{1}{Y_{X/S}} \frac{dX}{dt} - \frac{1}{Y_{P/S}} \frac{dP}{dt} \\ \frac{dP}{dt} &= \alpha \frac{dX}{dt} + \beta X \end{aligned} \quad (6)$$

with initial conditions $t = 0, X = X_0, S = S_0, P = P_0$.

With the aim of finding the best expression for specific biomass growth rate, all kinetic models listed in Table 1, as well as the modified logistic and Gompertz equations were used.

An algorithm for simultaneously solving the model equations describing the fermentation process at different initial substrate concentrations was developed.

Using this algorithm, own experimental data were used to identify the model parameters by least square function minimization using **MATLAB 2025** software.

For this purpose, the experimental data were processed by minimization procedure of the target function Q , being the sum of the squares of the differences between the measured biomass, substrate, and lactic acid concentrations and the model values:

$$Q(\mu_{\max}, k_S, k_P, k_i, X_{\max}, Y_{X/S}, \alpha, \beta, Y_{P/S}) = \frac{1}{N} \sum_{i=1}^N (X_i - X_i^{\text{exp}})^2 + \frac{1}{N} \sum_{i=1}^N (S_i - S_i^{\text{exp}})^2 + \frac{1}{N} \sum_{i=1}^N (P_i - P_i^{\text{exp}})^2 \rightarrow \min \quad (7)$$

where i is the number of constants in each equation for μ , and j is the number of experimental points.

The attempt to solve the model with the data for all 5 substrate concentrations wasn't very successful, the discrepancies between model and experimental data were large and the Q function value was too big.

Analyzing the data for product accumulation in Figure 1 it can be concluded that while at 11 g/L substrate concentration, the conversion is almost complete, while increasing the substrate concentration from 22 to 55 g/L leads to strong inhibition of the process and the conversion drops up to about 30%. It was decided to solve the model for 11 g/L separately, using an expression for μ without any additional terms for substrate and product inhibition. Four equations were used – the Monod equation, Verhulst equation, modified logistic, and modified Gompertz equations.

The results are shown in Figure 3, and the model parameter values are listed in Table 2. All four equations provided a good description of biomass growth, with the Gompertz and Verhulst equations giving the closest fit. However, when the full system of equations for biomass growth, substrate consumption, and product formation was solved simultaneously, the outcomes differed slightly: the Verhulst equation gave the best overall fit, while the Gompertz equation yielded a higher Q function value and larger discrepancies between model predictions and experimental data for substrate and product.

The calculated maximum cell concentrations ($X_{\max}$ and A) were very similar, as were several other model parameters. The lag phase was very short, with the modified Gompertz and logistic models predicting approximately 3–4 hours. The α and β parameter values indicate that lactic acid production by *L. plantarum* AC 11S is growth-associated, with almost no production occurring during the stationary phase.

Table 2. Model parameters determined by solving the system 6 for 11 g/L initial substrate concentrations

Model	$\mu_{\max}$	K_S	$X_{\max}$	λ	A	$Y_{X/S}$	$Y_{P/S}$	α	β	Q
Monod	0.420	5.511				0.175	4.016	5.965	0.0197	1.019
Verhulst	0.253		2.045			0.202	6.394	5.396	0.0077	0.352
Gompertz	0.048			2.959	1.925	0.205	5.986	6.086	0.0042	3.846
Logistic	0.138			4.0705	1.875	0.229	2.011	4.591	0.0	1.949

Four equations were used – the Monod equation, Verhulst equation, modified logistic, and modified Gompertz equations and the results are presented in Figure 2

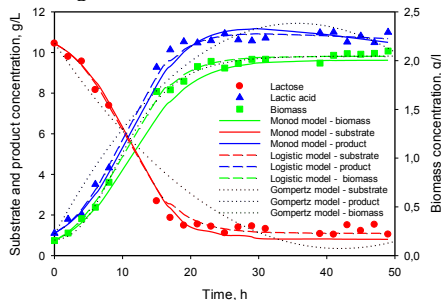


Figure 2. Experimental and model results for microbial growth, substrate consumption, and lactic acid production from 11 g/L initial substrate concentration.

For the rest of the experimental data (from 22 to 55 g/L initial substrate concentration) the mathematical model was solved with all equations that include different types of inhibition in the expressions for specific growth rate μ listed in Table 1.

The values of the parameters obtained after solving the mathematical model simultaneously for the three initial substrate concentrations are presented in Tables 3 and 4. The values of the maximum specific growth rate are very close but a little bit higher for the lactose as substrate. Comparing pH-controlled and pH-uncontrolled fermentations it may be seen that the values in controlled fermentations are slightly higher. The obtained values of $\mu_{\max}$ are very close to these reported in the literature for LA production from lactose [17, 18]. In all cases, the lactic acid fermentation was growth-related, which was confirmed by the ratio of the parameters α and β .

Table 3. Lactic acid fermentation without pH control.

Initial substrate concentrations (10, 20, 30 g/l)	Model parameters										
	$\mu_{\max}, h^{-1}$	$X_{\max}, g\ dm^{-3}$	n	$v_{x,s}, [-]$	$Y_{p,s}, [-]$	α, h^{-1}	β, h^{-1}	Q	R^2	RMSE	RSS
$S_{lactose}^0$	0.2402	2.2447	1.7068	0.1647	4.3034	6.3202	0.0029	3.150	0.994	1.775	13.60
S_{DOGS}^0	0.2309	1.3693	0.9693	0.1798	5.2371	7.9996	0.0136	2.871	0.996	1.694	23.13

Table 4. Lactic acid fermentation with pH control.

Initial substrate concentrations (10, 20, 30 g/L)	Model parameters										
	$\mu_{\max}, h^{-1}$	$X_{\max}, g\ dm^{-3}$	n	$v_{x/s}, [-]$	$Y_{P/S}, [-]$	α, h^{-1}	β, h^{-1}	Q	R^2	RMSE	RSS
S_{lactose}^0	0.2539	3.7727	1.8228	0.1715	4.7211	5.6631	0.0044	3.521	0.966	1.876	52.57
S_{DOGS}^0	0.2415	1.906	1.2517	0.2566	2.1982	7.2765	0.0133	0.403	0.992	0.635	33.75

The results of mathematical modeling are presented in Figures 3 and 4. There is not a statistically significant difference between experimental and model data. A very good agreement between experimental and computed results is observed.

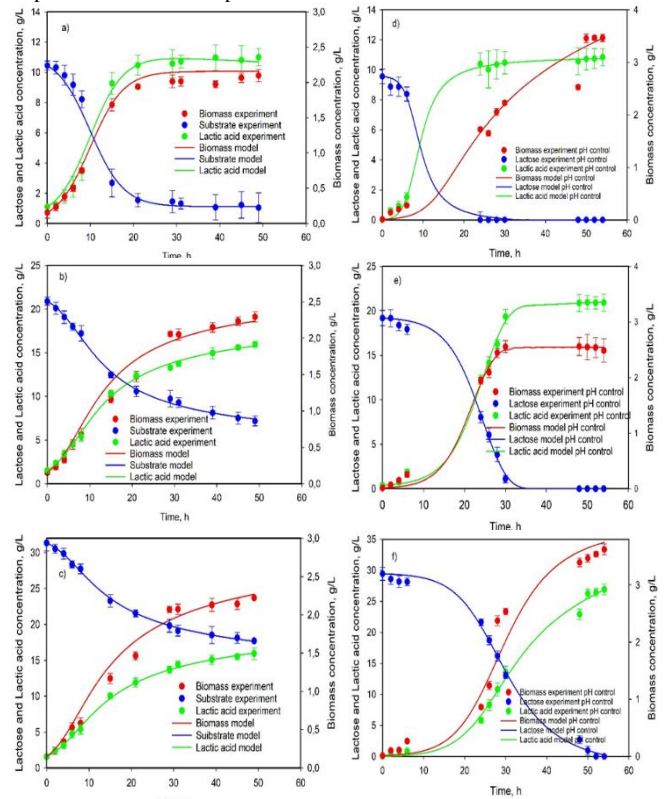


Figure 3. Modeling of biomass growth, lactose consumption, and lactic acid production a), b), and c) 10, 20, and 30 g/L without pH control; d), e), and f) 10, 20, and 30 g/L with pH control.

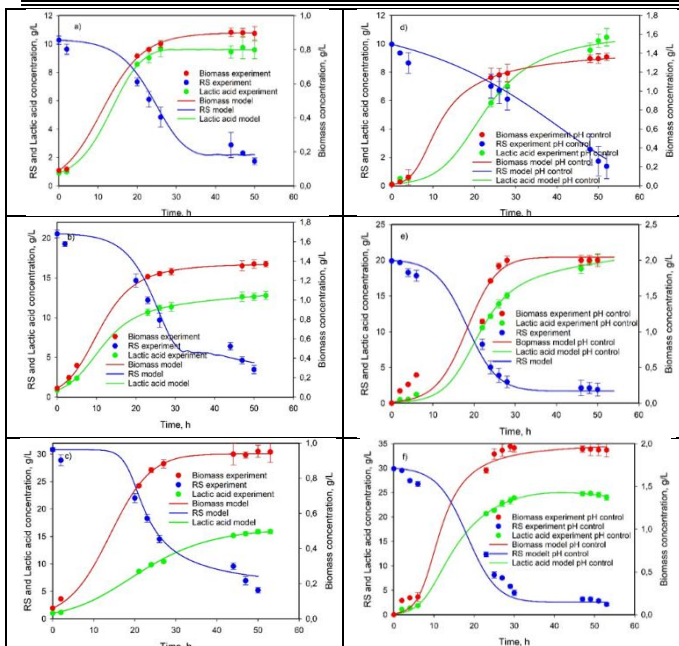


Figure 4. Modeling of biomass growth, substrate consumption, and lactic acid production from DDGS hydrolysates. a), b), and c) 10, 20, and 30 g/L RS without pH control; d), e), and f) 10, 20, and 30 g/L RS with pH control.

3.3. Model predictions.

A key advantage of applying suitable mathematical models to fermentation lies in their ability to predict system behavior under varying conditions. Once the model parameters were established, simulations were made to estimate the onset of inhibition and to assess lactic acid production at higher substrate concentrations. The model was tested using six initial substrate levels ranging from 11 to 22 g/L.

The model predictions are presented in Figure 5. From the inner picture, one can see that the inhibition starts between 15 and 16 g/L. The model was also solved for higher initial substrate concentrations – from 60 to 100 g/l and the results are presented in Figure 6.

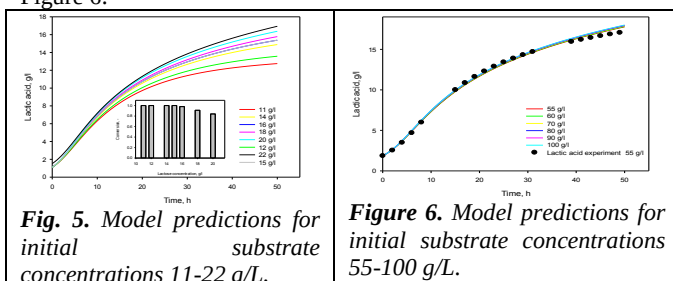


Fig. 5. Model predictions for initial substrate concentrations 11-22 g/L.

Figure 6. Model predictions for initial substrate concentrations 55-100 g/L.

4. Conclusions

This study investigates lactic acid production using lactose and divers DDGS hydrolysates as substrates. The resulting sugar solutions were fermented by *L. plantarum*, both with and without pH control, and the outcomes were compared to fermentations using lactose as a sole carbon source. Both types of fermentation were growth-associated. Implementing pH control improved lactic acid yields for both substrates, achieving complete conversion at initial substrate concentrations of 10 and 20 g/L, and 82–86% conversion at 30 g/L.

A mathematical model incorporating the Verhulst, Luedeking–Piret, and modified Gompertz equations was used to describe the experimental data, showing very good agreement. The parameter values obtained were consistent across all experiments and were higher in case of pH controlled process. These results provide a solid base for further studies on the strain's capabilities, which will include comparing model predictions with experimental results under pH-controlled conditions, as well as in fed-batch and continuous fermentation modes.

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Simulation of Inverse Dynamics Control of UAV with SIMULINK

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Abstract: Inverse dynamics control represents a robust methodology within the realm of nonlinear control system design. At its core, this approach involves constructing an inner-loop controller that leverages the motion characteristics of a nonlinear dynamic model. By systematically inverting the plant's dynamics, engineers can formulate control laws that effectively neutralize inherent nonlinearities, decouple complex variable interactions, and precisely shape the temporal behavior of task error convergence.

This article provides a comprehensive exploration of inverse dynamics control, emphasizing its practical implementations and the role of numerical techniques in solving the inverse dynamics problem. These computational methods are instrumental in translating theoretical models into robust controllers suitable for a wide range of engineering applications. The foundation of this approach lies in analytical mechanics, where control inputs are derived to enforce desired trajectories and system behaviors, ensuring both stability and performance.

Through dynamic model inversion, the control system can impose appropriate linear-like behavior on inherently nonlinear systems. This facilitates the design of controllers that are not only responsive but also adaptable to varying operational conditions. The technique proves especially valuable in scenarios involving complex mechanical and robotic systems, where precision and coordination are paramount.

Illustrative examples with SIMULINK underscore the versatility of inverse dynamics control. Applications range from robots operating under environmental constraints to systems with flexible joints and autonomous platforms that require synchronized motion. In each case, the inverse dynamics framework enables engineers to achieve high-fidelity control, even in the presence of structural complexity or external disturbances. Ultimately, inverse dynamics control serves as a cornerstone of modern control strategies, offering a structured framework for harnessing nonlinear dynamics in the service of predictable, efficient, and intelligent system behavior.

KEYWORDS: INVERSE DYNAMICS CONTROL, MODEL-BASED CONTROL, UAV, SIMULINK, NUMERICAL SOLUTION OF INVERSE DYNAMICS CONTROL.

1. Introduction

Unmanned aerial vehicles (UAVs) have become essential tools in modern engineering, offering versatility and precision in a variety of applications. The control of UAVs, especially those with nonlinear dynamics, presents significant challenges that require advanced methodologies. Inverse dynamics control stands out as a powerful approach, enabling engineers to design controllers that can effectively manage complex system behaviors. By leveraging mathematical modeling and simulation tools like SIMULINK, it is possible to develop robust control strategies tailored to the unique requirements of UAV platforms. This work focuses on the practical implementation of inverse dynamics control for a fixed-wing tandem UAV, highlighting the integration of analytical and numerical techniques.

2. Mathematical Model of the Fixed-Wing Tandem UAV for Inverse Dynamics.

Briefly, we will explain the mathematical model of tandem fixed wing since similar but different in some crucial details have been used in several places of the research below m and J – platform mass and inertia matrix in the body axes; $v^{(w)} = [1 \ 0 \ 0]^T v$ - vehicle inertial velocity representation in the wind axes; $\omega_w^{(w)}$ and $\omega^{(b)} = [P \ Q \ R]^T$ - representations of the wind axes angular velocity $\vec{\omega}_w$ and the aircraft(body axes) angular velocity $\vec{\omega}$ respectively in the wind and body axes; and $\tilde{\omega}$ - a skew-symmetric matrix associated with ω to represent the vector product in matrix notation, e.g., the product $\vec{\omega}_w \times \vec{v}$ is described in the path axes as $\tilde{\omega}_w^{(w)} v^{(w)}$. The applied forces and moments, $F^{(w)}$ and $M^{(b)}$, respectively, in the wind and body axes, are:

Forces and moments

$$\begin{aligned} (1) \quad m\dot{v}^{(w)} + m\tilde{\omega}_w^{(w)}v^{(w)} &= F^{(w)}; \\ (2) \quad J\dot{\omega}^{(b)} + \tilde{\omega}^{(b)}J\omega^{(b)} &= M^{(b)} \end{aligned}$$

$$(3) \quad F^{(w)} = -\frac{1}{2}\rho S v^2 \begin{bmatrix} c_D \\ c_S \\ c_L \end{bmatrix} + T \begin{bmatrix} \cos(\alpha + \alpha_T) \cos\beta \\ -\cos(\alpha + \alpha_T) \sin\beta \\ -\sin(\alpha + \alpha_T) \end{bmatrix} +$$

$$mg \begin{bmatrix} -\sin\gamma \\ \sin\phi\cos\gamma \\ \cos\phi\cos\gamma \end{bmatrix}$$

$$(4) \quad M^{(b)} = \frac{1}{2}\rho S v^2 \begin{bmatrix} b c_l \\ c_a c_m \\ b c_n \end{bmatrix} + T \begin{bmatrix} 0 \\ d \\ 0 \end{bmatrix} + J_T \omega_T \begin{bmatrix} -Q \sin\alpha_T \\ P \sin\alpha_T - R \cos\alpha_T \\ Q \cos\alpha_T \end{bmatrix}$$

The aerodynamic force and moment coefficients

$$\begin{aligned} c_D &= c_D(\alpha, \beta, \delta_e); \\ c_l &= c_l(\alpha, \beta, P, R, \delta_u, \delta_r); \\ c_S &= c_S(\alpha, \beta, P, R, \delta_r); \\ c_m &= c_m(\alpha, Q, \delta_e); \\ c_L &= c_L(\alpha, Q, \delta_e); \\ c_n &= c_n(\alpha, \beta, P, R, \delta_u, \delta_r); \end{aligned}$$

Designing Flight Control Laws: Once the UAV model was created in the SIMULINK, the next step was to design a longitudinal controller that commands elevator position to control altitude. The general nonlinear dynamics of the aircraft can be written as

$$(5) \quad \dot{x}(t) = f(x(t), \delta(t)) \quad (5)$$

Where the function $f()$ is assumed to be sufficiently smooth. The control input $\delta(t)$ is assumed to be bounded and piecewise continuous. The initial form of the inverse model could be written as follows, and of course, the model (7.1) should be invertible concerning $\delta(t)$

$$(6) \quad \delta(t) = \hat{f}^{-1}(x(t), v(t))$$

$$(7) \quad v(t) = \hat{f}(x(t), \delta(t)) \text{ Artificial control input}$$

An algorithm for calculating inverse dynamics and meeting the above requirements could be developed by using an artificial control input described in Equation (7.7):

$$(8) \quad \dot{x}(t) = v(x(t), \delta(t)) + \Delta(x(t), \delta(t))$$

Equation (7.10) is a pseudo-inverse version of Equation (7.5), and the next equation is the real one

$$(9) \delta(t) = g(x(t), \dot{x}(t))$$

$$(10) \delta(t) = g(x(t), f(x(t), \delta(t)))$$

Equation (10) is suitable for pure analytical solutions, which is somewhat unexpected. Equation 7.9 is more practical and can be used for both pure numerical solutions and semi-analytical solutions. Combining Equation 9 and Eq.10 is the best solution, which means that Eq.10 must be simplified enough without a lack of precision to be able to find an analytical-type solution of Eq.9.

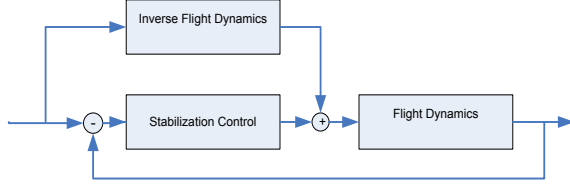


Figure 1: General Control Strategy for Inverse Dynamic Control

3. Mathematical Model of the Fixed-Wing Tandem UAV for Inverse Dynamics

u, v, w - body fixed linear velocity components in forward, side, and vertical directions, m/s;

$\dot{u}, \dot{v}, \dot{w}$ - linear accelerations, m/s²;

X_a, Y_a, Z_a - body forces per unit mass, N/kg;

p, q, r - body fixed roll, pitch, and yaw rates, degree/s;

g - acceleration due to gravity, m/s²;

$$(11) [\dot{x}_T, \dot{x}_m] = f(x_T, x_m, u) + d(x_T, x_m, u)$$

$$(12) \hat{x}_T = f(x_T, x_m, u) + \hat{d}(x_T, x_m, u) + K_2(x_T - \hat{x}_T)$$

Linear accelerations

$$(13) \dot{u} = rv - qw - g \sin \theta + X_a$$

$$(14) \dot{v} = pw - ru + g \sin \varphi \cos \theta + Y_a$$

$$(15) \dot{w} = qu - pv + g \cos \varphi \cos \theta + Z_a$$

Angular accelerations

$$(16) \dot{p} = C_3 L + C_4 N + C_2 pq + C_1 qr$$

$$(17) \dot{q} = C_7 M + C_6(p^2 - r^2) + C_5 pr$$

$$(18) \dot{r} = C_4 L + C_9 N + C_8 pq - C_2 rq$$

Where:

$$(19) C_1 = ((I_{yy} - I_{zz})I_{zz} - I_{xz}^2) / (I_{xx}I_{zz} - I_{xz}^2)$$

$$(20) C_2 = (I_{xx} - I_{yy} + I_{zz})I_{zz} / (I_{xx}I_{zz} - I_{xz}^2)$$

$$(21) C_3 = I_{zz} / (I_{xx}I_{zz} - I_{xz}^2)$$

$$(22) C_4 = I_{xz} / (I_{xx}I_{zz} - I_{xz}^2)$$

$$(23) C_5 = (I_{zz} - I_{xx}) / I_{yy}$$

$$(24) C_6 = I_{xz} / I_{yy}$$

$$(25) C_7 = 1 / I_{yy}$$

$$(26) C_8 = (I_{xx} - I_{yy})I_{xx} + I_{xz}^2 / (I_{xx}I_{zz} - I_{xz}^2)$$

$$(27) C_9 = I_{xx} / (I_{xx}I_{zz} - I_{xz}^2)$$

$\dot{p}, \dot{q}, \dot{r}$ - roll, pitch, and yaw angular acceleration

I_{xx}, I_{yy}, I_{zz} - Moments of inertia about x, y, and z axis, kg.m²

L, M, N - Roll, pitch, and yaw moments about body axis, N · m;

First derivatives of roll, pitch, and yaw:

$$(28) \dot{\theta} = q \cos \varphi - r \sin \varphi$$

$$(29) \dot{\varphi} = p + q \sin \varphi \tan \theta + r \cos \varphi \tan \theta$$

$$(30) \dot{\psi} = q \sin \varphi \sec \theta + r \cos \varphi \sec \psi \theta$$

Dynamics - The aerodynamic force and moment coefficients

$$(31) [X_a Y_a Z_a] = \frac{\bar{q} S}{m} [C_D C_Y C_L]$$

$$(32) [L M N] = \bar{q} S [b C_l c C_m b C_n]$$

C_l, C_m, C_n - roll, pitch, and yaw moment coefficients (rad)

C_D, C_Y, C_L - Drag, Lift, and Side forces coefficients

$\bar{q}$ = dynamic pressure, N/m²;

S = wing area, m²;

b = wing span, m;

c = chord length, m.

Forces coefficients

$$(33) C_L = C_{D0} + C_{L\alpha} \alpha + C_{L\delta_e} \delta_e + \frac{C_{Lq} q c}{2V}$$

$$(34) C_D = C_{D0} + K[C_L - C_{LminD}]^2 + C_{D\delta_e} \delta_e + C_{D\delta_a} \delta_a$$

$$(35) C_Y = C_{Y\beta} \beta + C_{Y\delta_a} \delta_a + \frac{[C_{Yp} p + C_{Yr} r] b}{2V}$$

Moment coefficients

$$(36) C_l = C_{l\beta} \beta + C_{l\delta_a} \delta_a + \frac{[C_{lp} p + C_{lr} r] b}{2V}$$

$$(37) C_m = C_{m0} + C_{m\alpha} \alpha + C_{m\delta_e} \delta_e + \frac{C_{mq} q c}{2V}$$

$$(38) C_n = C_{n\beta} \beta + C_{n\delta_a} \delta_a + \frac{[C_{np} p + C_{nr} r] b}{2V}$$

$C_{D0}, C_{L0}, C_{Y0}, C_{m0}$ - drag, lift, side force, and pitching moment coefficients at zero-angle of attack,

$C_{D\alpha}, C_{L\alpha}, C_{m\alpha}$ - drag, lift, and pitching moment coefficients at zero aoa

δ_a, δ_e - Aileron and elevator deflections

α, γ - aoa and flight path angle

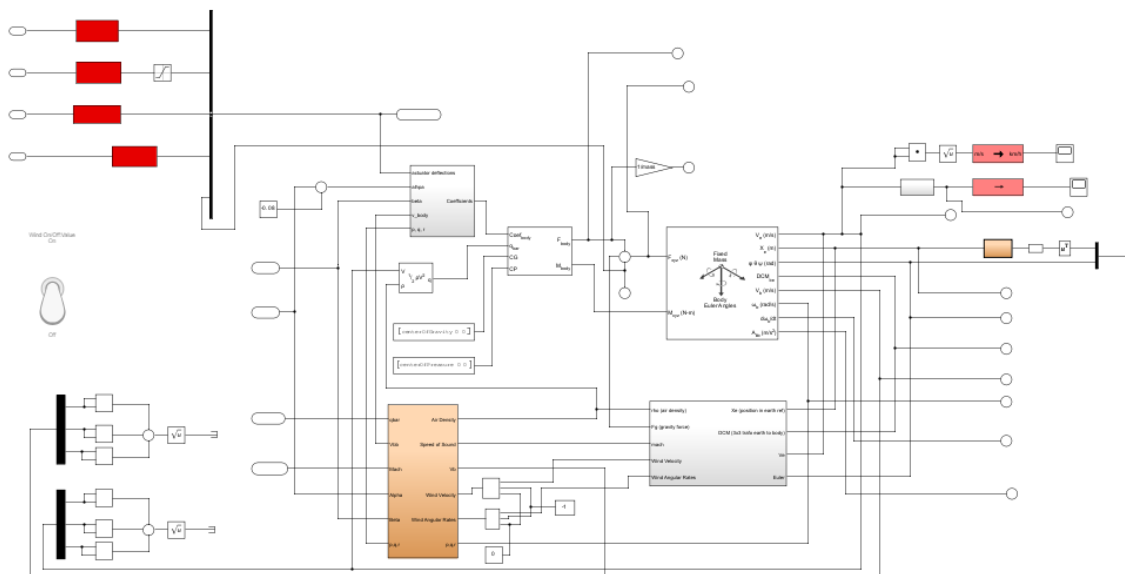


Figure 2: Simulink Block Diagram of the Inverse Dynamics Control System for a Fixed-Wing Tandem UAV

4. Acknowledgement

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Modelling of LTL routes for eco-diversed transport application

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Abstract:

This study addresses the vehicle routing problem (VRP) for eco-diverse transport fleets, defined as fleets comprising vehicles with heterogeneous engine systems, resulting in varied payload capacities, access restrictions, and levels of cost-efficiency and environmental performance. The research is driven by the growing integration of alternative fuel vehicles (e.g., electric and hydrogen-powered) into conventional transport fleets, coupled with the implementation of Clean Transport Zones (EcoZones) that impose access restrictions on combustion (diesel) vehicles. A two-stage, highly scalable bi-objective optimization algorithm is proposed, evaluated using a real-world case study involving the distribution of 356 pallets across 188 destinations within an approximate 140 km radius of Kielce, with 25% of these destinations located in potential EcoZone areas. The analysis assesses feasibility, ecological and economic cost intensity, and workload distribution across fleet segments under energy and access constraints. The developed algorithm demonstrates significant potential for prescriptive analytics in optimizing routing strategies amid the energy transition in the transportation sector.

KEYWORDS: ECO-DIVERSE FLEET, LTL TRANSPORT, VRP, MULTI-OBJECTIVE OPTIMIZATION, ITERATED LOCAL SEARCH, SIMULATED ANNEALING

1. Introduction

The transportation sector is undergoing a profound transformation, driven by the need to enhance sustainability while maintaining operational efficiency. This shift necessitates innovative approaches to the management, coordination, and performance evaluation of vehicle utilization. A key challenge in this domain is optimizing less-than-truckload (LTL) transport, where cost efficiency is achieved through advanced routing strategies and sophisticated algorithms [1]. These strategies aim to develop feasible, cost-effective, and environmentally sustainable route plans that balance economic and ecological objectives, as exemplified by the Pollution-Routing Problem (PRP) or Green Vehicle Routing Problem (Green VRP) [2,3]. Over recent decades, the Vehicle Routing Problem (VRP) has been extensively studied, giving rise to several variants, including the Capacitated VRP [4], the Time-Windowed VRP [5], and the Multi-Depot VRP [6]. The increasing diversity in order volumes and customer requirements has spurred the adoption of heterogeneous fleets, which combine vehicles with varying capacities and characteristics to meet operator's demands [7,8]. In recent years, the integration of electric vehicles (EVs) into VRP frameworks has gained significant attention [9–12]. These studies introduce additional constraints, related to the limited energy capacity of EVs, which necessitates innovative solutions such as incorporating full or partial battery charging into route planning to mitigate range limitations [13]. Alternatively, scheduled battery-swapping procedures have been proposed as a viable approach to enhance operational feasibility [14,15]. A particularly promising strategy is the mixed (eco-diversed) fleet approach, which combines conventional diesel vehicles with eco-friendly battery electric vehicles (BEVs) [16]. This approach offers a pragmatic solution, aligning with global imperatives to reduce greenhouse gas emissions while preserving fleet transport capacity.

This study concentrates on the field of sustainable transportation by developing and evaluating optimized routing strategies for mixed-fleet operations. The primary contribution lies in the design and implementation of a prototype fleet management system that integrates a novel planning–optimization module tailored for eco-diverse fleets. This module employs a bi-objective optimization algorithm with an inter-criteria balancing function, enabling the identification of routing solutions that are feasible under energy and access constraints while minimizing both economic costs and negative environmental impact. To demonstrate the practical

applicability of the proposed system, the study conducts a comprehensive analysis using a real-world case study involving the distribution of 356 pallets across 188 destinations. The analysis evaluates key performance metrics, including feasibility, ecological and economic cost intensity, and workload distribution segments, as functions of imposed energy constraints and access restrictions (e.g. EcoZones). By quantifying the trade-offs between economic and environmental objectives, this work provides actionable insights for logistics operators seeking to transition to sustainable fleet management practices.

2. Optimization Algorithm and Model

The analysis of routing strategies for eco-diverse heterogeneous resources was carried out using a proprietary planning algorithm developed within the research and development project TRAFFIC (Towards Route Autopanning for Eco-diverse Fleet and Flow Management with Improved Coordination). The TRAFFIC system is primarily intended for companies providing LTL transport services in the context of deterministic delivery and demand scenarios. To solve the routing problem, a custom two-stage algorithm was applied, combining a pseudo-greedy heuristic of the Nearest Neighbour (NN) type [17] with an evolutionary Iterated Local Search (ILS) metaheuristic [18].

The general structure of the method is shown in Fig. 1. The algorithm assigns orders from the *Requests* list to the resource base stored in *TruckList*, using sets of inter-distance, inter-time, and eco-distance matrices, along with the characteristics of the destination list *DestPos*.

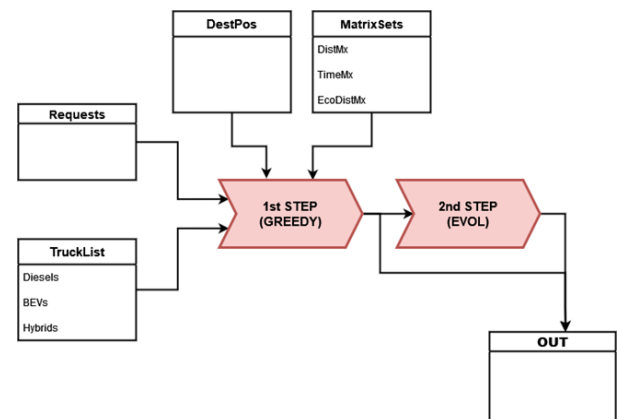


Fig. 1. Structure of the planning algorithm

The first stage of the planning algorithm (GREEDY) is deterministic in nature and is responsible for generating an initial, feasible, and quasi-optimal solution, by default engaging the smallest possible number of transport resources. In the second phase of the optimization procedure, a proprietary algorithm named EVOL was applied, based on iterated random mutations of feasible solutions. The primary optimization criterion of the EVOL phase is a generalized monetary cost function, defined as the sum of three components: the fixed cost associated with engaging a vehicle, the time-related cost, and the energy-related cost. The monetary cost generated by the i -th resource (vehicle) is expressed by Equation 1.

$$c_i = c^F_i + t_i \cdot u^h_i + e_i \cdot u^e_i \quad (1)$$

where:

c_i - total cost of the i -th resource

c^F_i - fixed cost of the i -th resource

u^h_i, u^e_i - unit monetary costs for Staff and Energy, respectively

t_i - total time engagement of the i -th resource

e_i represents the energy resources consumed by the i -th resource.

In the developed model, it is calculated based on the traveled distance d and the required time t , taking into account the load weight of the resource (Equation 2).

$$e_i = \sum_{k \in \tau_i} [d_{i,k} \cdot (\beta^c_i + \beta^v_i \cdot m_{i,k}) + t_{i,k} \cdot \beta^t_i] \quad (2)$$

where:

τ_i - route of the i -th resource

$\beta^c_i, \beta^v_i, \beta^t_i$ - unit costs (energy consumption per unit length, mass, and time)

$m_{i,k}$ - load of resource i at the k -th point of the route

$d_{i,k}, t_{i,k}$ - distance and time to cover the k -th segment of the route

The consumption of energy resources e_i simultaneously affects the value of the so-called ecological cost, which becomes an additional, independently treated optimization criterion. Ultimately, the developed optimization algorithm is guided by the criteria of minimizing both monetary cost and ecological cost:

$$\min_{i \in \Pi} c_i \quad \min_{i \in \Pi} e_i \cdot u^c_i \quad (3)$$

where: Π - the set of resources, u^c_i - the unit ecological cost (CO₂ emissions per unit of energy).

The following constraints are imposed on the set of routes τ_i regarding total mass (MassLimit), volume (VolLimit), energy consumed (EnergyLimit), allowable resource activity time (MaxActivityTime), and maximum time of a single trip (MaxTripTime).

$$\bigwedge_{i \in \Pi} \sum_{k \in \tau_i} m_{i,k} < \text{MassLimit}_i \quad (4a)$$

$$\bigwedge_{i \in \Pi} \sum_{k \in \tau_i} v_{i,k} < \text{VolLimit}_i \quad (4b)$$

$$\bigwedge_{i \in \Pi} e_i < \text{EnergyLimit}_i \quad (4c)$$

$$\bigwedge_{i \in \Pi} t_i < \text{MaxActivityTime}_i \quad (4d)$$

$$\bigwedge_{i \in \Pi} \bigwedge_{j \in \tau^p_{i,j}} \sum_{k \in \tau^p_{i,j}} t_{j,k} < \text{MaxTripTime}_i \quad (4e)$$

where: $\tau^p_{i,j}$ - a single trip performed by the i -th resource

In the presence of EcoZone Θ_e an additional condition is a restriction on access for vehicles that do not meet the criteria. This means that each point k of the route τ_i must be accessible by a resource belonging to the set Π_e of eco-friendly vehicles.

$$\bigwedge_{k \in \tau_i, \Theta_e} i \in \Pi_e \quad (5)$$

The EVOL algorithm also incorporates the concept of simulated annealing [15], which involves conditionally accepting mutations characterized by a negative threshold, whose value is relaxed to zero during the evolution process. The algorithm performs a specified number of MaxIters iterations. The acceptance criterion (Acc) for the considered criterion in the current iteration $iter$ is expressed by the following formula:

$$\text{Acc}(iter) = \begin{cases} 1 & \text{if } \Delta c < s_0 \cdot \left(1 - \frac{iter}{\text{MaxIters}}\right)^2 \cdot R_{iter} \\ 0 & \text{otherwise} \end{cases} \quad (6)$$

where:

s_0 - initial relative acceptance threshold,

Δc - cost change in the current iteration

R_{iter} - reference threshold, dynamically updated according to the formula:

$$R_{iter} = \rho \cdot |\Delta c_{iter}| + (1 - \rho) \cdot R_{iter-1} \quad (7)$$

ρ - exponential filter coefficient.

In general, the algorithm is guided by a two-criteria cost measure, with independent acceptance conditions determined for each criterion (economic and ecological). To make the algorithm more flexible, the concept of probabilistic relaxation of conditions was introduced, represented by the *balance* coefficient, which belongs to interval $<0-1>$. The determination of the acceptance condition (TotAcc) in the weighted bi-criteria variant is calculated according to the general formula (8).

$$\text{TotAcc} = (\text{Acc1} \vee \text{rnd}(1) < w_1) \wedge (\text{Acc2} \vee \text{rnd}(1) < w_2) \quad (8)$$

where: *Acc* - a binary variable defining whether a given criterion is met, *rnd*(1) - a randomly selected number from the range 0–1, and w_1 and w_2 are determined from the value of *balance*. When *balance* = 0, the ecological criterion is always accepted; in this case, the algorithm operates under single-criterion optimization conditions (SOCO - Single Objective Combinatorial Optimization). When *balance* = 0.5, a mutation is accepted only if the both *Acc* are simultaneously satisfied, and the algorithm operates in the bi-criteria regime (BOCO - Bi-Objective Combinatorial Optimization).

The planning algorithm was implemented in Mathcad PRIME 8.0. Analyses were carried out on an MSI Notebook, model MS179F, equipped with an Intel(R) Core(TM) i7-8750H CPU @ 2.20GHz and 8 GB RAM.

3. Results and discussion

3.1. Case description

The considered model case for the routing strategy assumes the delivery of 356 pallets to 188 destinations using a capacity-homogeneous, eco-diverse fleet. The order parameters are presented in Table 1.

Table 1. General characteristics of orders

Parametr	
Number of destinations	188
Average distance from base to destination	58.7km
Max. distance from base to destination	138.8km
Total order volume	356 pallets
Size of a single order	1 – 4 pallets
Average order volume	~1.9 pallets
Volume to eco-zones	89 pallets (25%)
Weight of a single pallet	400kg

The order size ranges from 1 to 4 pallets, with 25% of the orders directed to the EcoZone area. The destinations are dispersed over an area of nearly 50,000 km², with a certain tendency toward natural clustering. The maximum distance from the depot to a destination was 138 km, the minimum was less than 1 km, and the average distance was approximately 57 km. Real distance and travel time parameters were obtained from geographic information systems in the manner presented in [19]. In the considered case, the presence of two types of vehicles with identical transport capacities was assumed, differing in the type of drive: Diesel and BEV – Table 2. The parameters of energy resource consumption were estimated based on vehicle manufacturers' data, own observations, and observations from transport companies carried out within the TRAFFIC project.

Table 2. General characteristics of vehicles

Parameter	Diesel	BEV (Mixed1)	BEV (Mixed2)
Trucks	28	12	
EnergyLimit	100 dm ³	100 kWh	200 kWh
MaxTripTime	8 h		6 h
InterTrip Time	0.5 h		2.5 h
$\beta^c_{i'}$	10 dm ³ /100km	35 kWh/100km	
$\beta^v_{i'}$	1.3 dm ³ /100km/t	4.5 kWh/100km/t	
β^t_i	1 dm ³ /1h	3.5 kWh/1h	
u^e	1.5 Euro/ dm ³	0.5 Euro/kWh	
c^F	50 Euro	75 Euro	
u^c	2.5 kg/ dm ³	0.25 kg/kWh	
u^h	10 Euro/h		
VolLimit	10 pallets		
MassLimit	10Mg		
MaxActivityTime	12h		
LoadUnit Time	6 min/pallet		

The parameter values indicate a clearly higher economic cost and, at the same time, a lower ecological cost for the BEV segment. Two cases differing in the ability to replenish energy resources were analyzed. In the Mixed1 case, it was assumed that recharging during the MaxActivity Time is not possible. In the Mixed2 case, it was assumed that a one-time replenishment of energy resources is possible, which translates into a twofold increase in the energy resource limit, a reduction of the maximum trip duration (MaxTripTime) by 2 hours, and an increase in InterTrip Time by 2 hours respectively.

3.2. Migration to ecodiversed fleet

It was demonstrated that neither a fully combustion-engine fleet nor a fully electric fleet is capable of fulfilling all orders. In the case of the combustion-engine fleet, 25% of orders were not serviced due to the presence of clean transport zones. In the case of the fully electric fleet, approximately 7.6% of the order volume was not serviced due to excessive distance from the base to the destination. Full order coverage, however, is ensured by an eco-diverse fleet. In the further part of the study, a hypothetical reference case (Diesel-Only) was also considered, involving only a traditional fleet under conditions without the EcoZones.

Table 3 presents the calculated cost-intensity and energy-intensity parameters of the solutions for the Mixed1 and Mixed2 fleets, compared to the reference case (Diesel-Only). The differences in terms of total distance traveled, time-intensity, and the number of required trips for each of the three cases are statistically insignificant. Therefore, distance is not a reliable parameter for differentiating between the analyzed cases. As a

result, the differences in cost-intensity of the solutions are mainly due to differences in the Fix Cost of fleet maintenance.

Table 3. Cost-intensity and energy-intensity parameters of the solutions for the respective fleet variants.

PARAMETER	Diesel-Only	Mixed1	Mixed2
Total Distance [km]	5311.22	5323.70	5308.24
Total Monetary Cost [euro]	3431.83	3716.22	3657.03
Energy Cost [euro]	1152.61	1189.44	1185.10
Staff Cost [euro]	1489.22	1489.29	1486.93
Fix Cost [euro]	790	1037.5	985
Total Fleet Volumen [pallets]	158	177	172
Trips	36	36.2	36.2
Total Activity Time [h]	159.02	158.18	159.99
CO2 emmission [kg]	1921.01	1689.93	1684.99
Trucks needed	16	18	17-18

The transition to an eco-diverse fleet may require equipping it with a set of at least 6 BEV-type vehicles, while reducing the number of traditional vehicles by up to 4. Under conditions allowing recharging, the minimum number of BEV-type vehicles is 5. The analysis shows that migration to eco-diverse fleets is associated with an approximately 31% increase in fixed costs in the case of Mixed1 and about 25% in the case of Mixed2. At the same time, this leads to a reduction in CO₂ emissions of around 12%.

Subsequently, the activity time of individual resources (Truck Activity Time), resulting from the generated route plan, was analyzed. The load includes transshipment time as well as potential BEV vehicle recharging. The load of the reference fleet's vehicles (Diesel-Only) ranges from 7.4 to 11.77 hours – Fig. 2. In the case of the Mixed1 fleet, a noticeably lower load of the BEV segment is observed – an average vehicle of this type was engaged for only 5.8 hours, which is a consequence of limiting energy resources to 100 kWh.

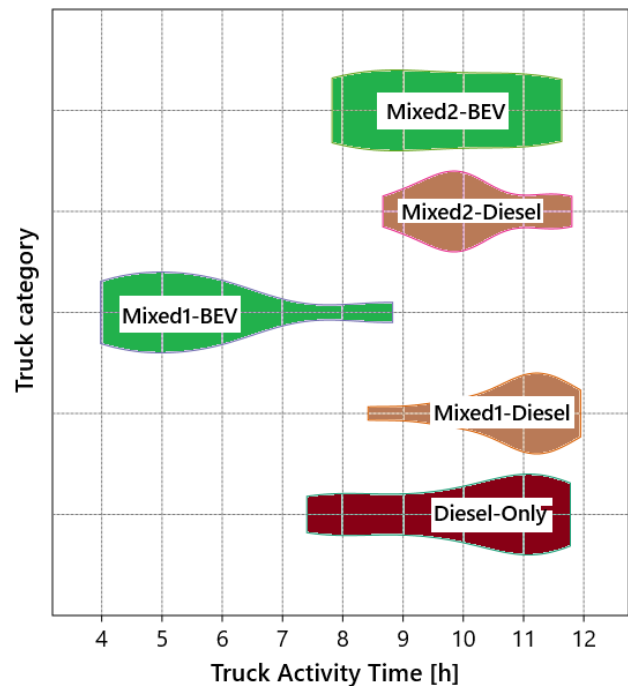


Fig. 2. Activity time of individual resource categories in the respective fleet variants

Under conditions allowing recharging, the activity of vehicles does not differ from the engagement level of the combustion-engine segment. A significant reduction (from 61 to 50 pallets) in the required total average volume of the BEV segment was observed. At the same time, no statistically significant difference was noted between the Mixed1 and Mixed2 fleets in terms of distance traveled, energy cost, or total cost. However, the benefits resulting from the reduction of fleet resources are offset by the increased fleet activity time (higher labor cost) caused by the time-consuming charging process.

3.3. Participation of the BEV segment in transport service delivery – SOCO vs. BOCO optimization

The participation of the BEV segment in the Mixed1 and Mixed2 fleets was analyzed in relation to various planning solution parameters, including the percentage of serviced orders, share in operating costs, distance traveled, and process time intensity. A series of routing optimizations was carried out in a single-criterion variant (monetary cost – SOCO) and a dual-criterion variant (monetary cost and CO₂ emissions – BOCO). The results are shown in Figure 3.

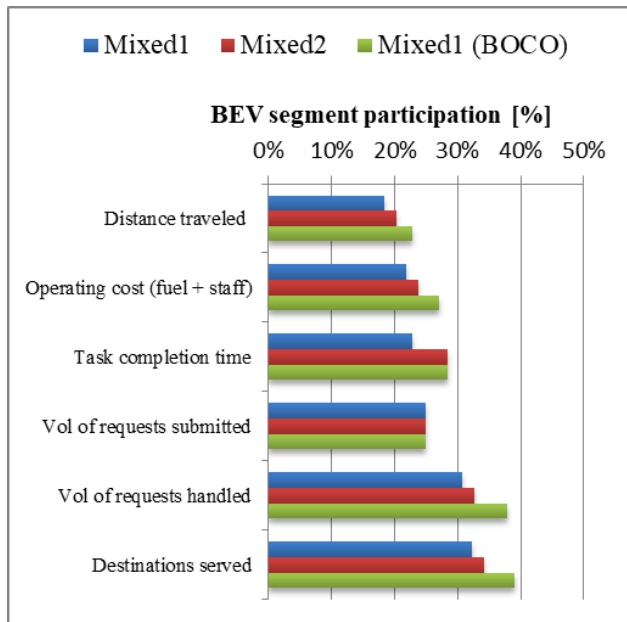


Fig. 3. Participation of the BEV segment in various planning solution parameters

In terms of the volume of serviced orders and visited destinations, the share of the BEV segment was clearly greater than that resulting from the share of the EcoZone. In the BOCO variant, electric vehicles serviced approximately 39% of destinations and delivered 135 out of 356 pallets (37.7%). This results from the optimization algorithm's tendency to minimize ecological cost, which favors BEV-type vehicles. In this latter case, 7 out of 12 (nearly 60%) deployed BEV vehicles were used, whereas Diesel vehicle utilization amounted to no more than 12 out of 28 (just over 40%). On the other hand, the BEV vehicles' share in the total distance traveled was relatively small. In the case of the Mixed1 fleet, these vehicles covered only about 18.4% of the total distance, while their share of the transport volume was over 34%. This is related to the imposed limitations on energy resources, which forces the algorithm to assign BEV vehicles to trips involving destinations located closer to the starting point (depot).

4. Conclusion

The study presented a detailed analysis of the costs of eco-diverse mixed fleets operating in a less-than-truckload transport regime. The analysis was conducted for a representative case of delivering 356 pallets to 188 delivery points, subject to access restrictions resulting from local conditions and the hypothetical location of so-called clean transport zones. It was shown that mixing the fleet may be a necessary requirement to achieve 100% capability to meet transport demands. In the considered case, full replacement of the combustion-engine fleet with a mixed fleet led to an increase in transport service cost of approximately 8.3%, resulting mainly from the higher purchase and maintenance costs of electric vehicles. No significant increase was observed in staff costs or energy costs. On the other hand, CO₂ emissions were reduced.

5. Acknowledgements

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ЭФФЕКТИВНОСТЬ ТЕХНОЛОГИЧЕСКИХ СХЕМ АСИММЕТРИЧНОЙ ПРОКАТКИ В РЕЛЬЕФНЫХ ВАЛКАХ

EFFICIENCY OF TECHNOLOGICAL SCHEMES OF ASYMMETRIC ROLLING IN RELIEF ROLLS

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Abstract: This paper presents the issue consideration results of obtaining thick-sheet blanks with an increased processing level. Based on the review conducted in this paper, a new technology of thick-sheet rolling was proposed, which consists in deforming the workpiece in rolls with a relief surface that have a geometric or velocity factor of asymmetry. As a result, shear strain in both transverse and longitudinal directions is intensified in one pass. Finite element modeling of the microstructure evolution of a copper billet during asymmetric rolling in relief rolls according to various technological schemes was performed. The following technological schemes of deformation were proposed: 1) the workpiece after the first pass of deformation is re-fed into relief rolls with 180° edging along the axis; 2) the workpiece after the first pass of deformation is re-fed into relief rolls without any changes; 3) the workpiece after the first pass of deformation is re-fed into relief rolls with a transverse shift for the relief period. A comparison of the simulation results showed that deformation with a 180° rotation of the workpiece between passes significantly reduces the influence of the asymmetry factor. This is reflected in the level of grain refinement and more uniform distribution. Deformation without changing the position of the workpiece between the passes has the opposite effect, such a scheme significantly increases the influence of the asymmetry factor. Deformation with transverse shift of the workpiece for the relief period between passes has the effect of a "golden mean".

Keywords: ROLLING, RELIEF ROLLS, ASYMMETRY, SIMULATION, MICROSTRUCTURE EVOLUTION.

1. Введение

Одним из перспективных методов интенсивной пластической деформации, применяемых в промышленности, является асимметричная прокатка [1, 2]. Прокатка - сложный технологический процесс, сопровождающийся неровностями, поэтому любой процесс прокатки является асимметричным. Симметричная прокатка - это идеализация реальных условий. Однако асимметрия может быть создана целенаправленно из-за несоответствия окружных скоростей валков при использовании индивидуального привода, разницы в диаметрах валков и использовании не приводимого в движение (холостого) валка. В дополнение к использованию фактора асимметрии, который приводит к возникновению деформации сдвига в продольном направлении, были также рассмотрены наиболее эффективные методы прокатки, которые создают деформацию сдвига в поперечном направлении.

В работе [3] была разработана энергосберегающая технология прокатки толстолистового металла, которая решила проблему получения высококачественного толстолистового металла без существенного изменения исходных размеров заготовки. Для этого были разработаны две новые конструкции рабочих валков с рельефными поверхностями в виде кольцевых каналов, образующих трапециевидные выступы и впадины, чередующиеся один за другим по всей длине бочки.

В результате объединения этих двух схем с учетом коэффициента асимметрии были получены следующие новые схемы прокатки:

1) асимметричная прокатка в радиусных валках. Техническим результатом, получаемым с использованием данной схемы, является возможность создания благоприятного напряженно-деформированного состояния в металле для улучшения качества прокатываемого толстого листа за счет реализации значительных сдвиговых деформаций при прокатке, как в поперечном, так и в продольном направлениях, обеспечивая интенсивное измельчение исходного размера зерна и избегая появления опасных концентраторов напряжений в процессе прокатки, которые могут привести к разрушению металла. Это достигается за счет того, что предлагаемые валки для прокатки толстых листов включают в себя верхние и нижние валки с рельефной поверхностью в виде кольцевых буртиков и потоки, чередующиеся по всей длине бочки валка, с радиусом профиля потока, равным радиусу профиля буртика, в котором диаметр прокатки диаметр

нижнего валка в 1,5 раза больше диаметра прокатки верхнего валка. Наличие рельефной поверхности на валках и 1,5-кратное соотношение между диаметром прокатки нижнего валка и диаметром прокатки верхнего валка обеспечивает развитие дополнительной деформации сдвига как в поперечном, так и в продольном направлениях заготовки. А тот факт, что рельефная поверхность верхнего и нижнего валков выполнена в виде кольцевых буртиков и потоков, чередующихся по всей длине бочки валка, с радиусом профиля потоков, равным радиусу профиля буртиков, позволит создать дополнительную деформацию сдвига. реализуется в металле без появления опасных концентраторов напряжений и, соответственно, без разрушения металла.

2) асимметричная прокатка в рельефных валках (рис. 1). По аналогии с радиусными валками, в данном случае также использовался коэффициент геометрической асимметрии 1,5. Обработка в поперечном направлении становится более интенсивной из-за наличия трапециевидных выступов, смещение которых оказывает более выраженный эффект, но менее равномерное, как в радиусных валках.

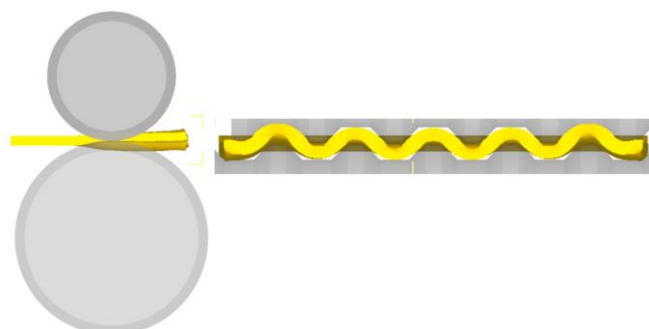


Рис. 1. Асимметричная прокатка в рельефных валках

2. Методика

Разработанный процесс интенсивной пластической деформации, представляющий собой комбинацию прокатки в рельефных валках с введением коэффициента асимметрии, хорошо зарекомендовал себя на теоретическом этапе исследований. Так, в работах [4, 5] были изучены различные параметры процесса с использованием кинематической и геометрической асимметрии. Энергосиловые параметры этой схемы деформирования также были рассмотрены в работе [6].

Анализ параметров напряженно-деформированного состояния показал, что одного цикла деформирования (прокатки заготовки в рельефных валках и выравнивания в гладких валках до первоначальной формы) недостаточно для качественной обработки металла. При многоходовой деформации обычно исследуется влияние количества проходов на уровень обработки и изменение исходного размера зерна. Однако такой подход к прокатке оправдан в случае симметричной нагрузки от обоих валков. В рассматриваемой схеме прокатки целесообразно рассмотреть различные технологические схемы деформирования, которые будут учитывать влияние фактора асимметрии. В соответствии с этим были предложены следующие технологические схемы деформирования:

- 1) после первого прохода заготовка повторно подается в валки с поворотом вдоль оси на 180 градусов;
- 2) после первого прохода заготовка повторно подается в валки без каких-либо изменений;
- 3) после первого прохода заготовка повторно подается в валки с поперечным сдвигом на период рельефа.

Основными характеристиками, использованными при изготовлении валков, были размеры канавки на корпусе валков. Угол наклона камеры был принят равным 45°. Расстояние между выступом одного валка и противоположной впадиной другого валка составляет 10 мм. Минимальное расстояние между скосами двух валков составляет 10 мм. Ширина бортиков - 10 мм. Радиус валка - 100 мм. Ширина валков - 190 мм. Построение моделей заготовки и толкателя выполнялось в программе DEFORM, где можно создавать простые трехмерные модели. Длина заготовки составляет 200 мм, ширина - 140 мм, а высота - 10 мм. В качестве исследуемого материала была выбрана медь. В программе DEFORM есть база данных материалов, из которых был выбран сплав C11000, поскольку он наиболее точно соответствует сплаву M1. Моделируемый процесс прокатки является холодным, поэтому температура заготовки и штампов устанавливается равной 20°C. Коэффициент теплопередачи был установлен равным 50 Вт/(м²×К). Расчет коэффициента теплопередачи излучением в окружающую среду проводился автоматически с учетом средних показателей шероховатости поверхности. Коэффициент трения для валков был установлен равным 0,45. В случае асимметричной прокатки скорость одного валка была установлена на 50% выше скорости другого, поэтому скорость вращения была установлена равной 90 об/мин для первого валка и 60 об/мин для второго. При симметричной прокатке скорость вращения двух валков составляла 60 об/мин.

3. Результаты и обсуждение

Для оценки эффективности технологических схем деформирования в качестве ключевого параметра обработки рассматривалась эквивалентная деформация, а также изменение исходного размера зерна, установленного на 100 мкм. В системе Deform традиционным методом моделирования эволюции микроструктуры является классический метод Джонсона-Мела-Аврами-Колмогорова (ЖМАК). В методе ЖМАК конечный средний размер зерна определяется на основе исходного среднего размера зерна, констант материала и переменных полей данных, таких как температура, деформация, скорость деформации и время. На рисунках 2-4 показаны графики эквивалентной деформации и распределения зерен по размерам по заготовке после двух проходов для трех рассматриваемых технологических схем деформирования. Здесь точки 1 и 3 соответствуют зонам поверхности, а точка 2 - осевой зоне. При повороте заготовки на 180° обе горизонтальные грани последовательно соприкасаются с каждым валком. В результате влияние фактора асимметрии минимально, поскольку каждая грань поочередно соприкасается с валком большего диаметра. Это хорошо видно при рассмотрении значений эквивалентной деформации при каждом проходе. После первого прохода (этап 3) и после второго прохода (этап 6) разница деформаций между зонами

поверхности уменьшается до 0,15. При этом максимальный уровень деформации составляет 2,4, а минимальный - 1,93 (рис. 2а). Рассматривая эволюцию микроструктуры после двух проходов (рис. 2б), было обнаружено, что распределение зерен по размерам имеет характерный полосатый вид, чередующийся в поперечном сечении заготовки. Средний размер зерен в наиболее развитых районах составляет 35 мкм, а в наименее развитых - примерно 65 мкм.

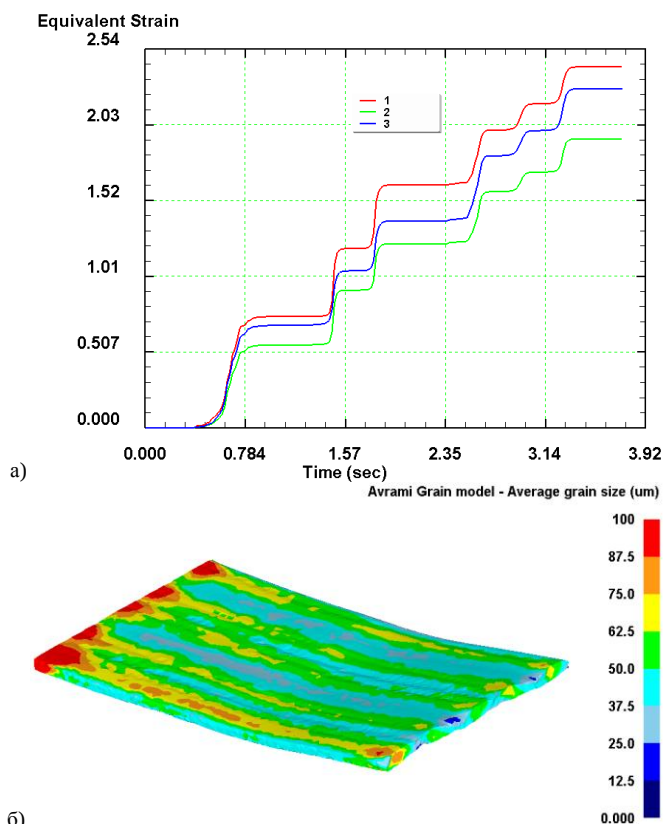


Рис. 2. Эквивалентная деформация (а) и эволюция микроструктуры (б) после двух проходов с поворотом заготовки на 180° между проходами

При деформировании без изменения положения заготовки происходит двойной идентичный контакт заготовки и валков. В результате влияние фактора асимметрии максимально, поскольку каждая грань соприкасается только с одним валком и только с определенной зоной рельефа. Это приводит к тому, что разница в значениях эквивалентной деформации после первого прохода (стадия 3) значительно возрастает до 0,6 после второго прохода (стадия 6). При этом максимальный уровень деформации составляет 3,5, а минимальный - 2,6 (рис. 3а). Учитывая эволюцию микроструктуры после двух проходов (рис. 3б), было обнаружено, что деформация без изменения положения заготовки приводит к существенной разнице в размерах зерен на исследуемых участках. Средний размер зерен на наиболее развитых участках составляет 25 мкм, а на наименее развитых участках - приблизительно 85 мкм.

При деформировании со сдвигом заготовки на период рельефа возникает двойной контакт между заготовкой и валками, однако при этом каждая грань соприкасается с разными зонами рельефа. В результате влияние коэффициента асимметрии довольно велико, но разница в эквивалентной деформации не увеличивается, оставаясь на уровне 0,4. При этом максимальный уровень деформации составляет 2,8, а минимальный - 2,3 (рис. 4а). Учитывая эволюцию микроструктуры после двух проходов (рис. 4б), было обнаружено, что деформация с поперечным смещением заготовки на период рельефа приводит к более равномерному распределению зерен по ширине заготовки. Средний размер зерен в наиболее развитых областях составляет 30 мкм, а в наименее развитых областях он составляет приблизительно 50 мкм.

4. Выводы

Сравнение технологических схем деформирования показало, что выбор схемы будет зависеть от желаемого результата, т.е. от требуемого уровня однородности свойств по сечению. В то же время необходимо отметить определенные особенности практической реализации каждой схемы. Деформация при повороте заготовки на 180° между проходами значительно снижает влияние фактора асимметрии. Это отражается на уровне эквивалентной деформации и ее разнице по высоте заготовки. Выбор данной схемы деформирования для практической реализации будет связан с дополнительной операцией поворота заготовки на 180° вдоль оси прокатки, для чего потребуется вспомогательное оборудование. Деформация без изменения положения заготовки между проходами имеет обратный эффект, такая схема значительно увеличивает влияние фактора асимметрии. Реализация этой схемы является наиболее простой, поскольку не требует каких-либо дополнительных операций или оборудования. Деформация с поперечным смещением заготовки на период рельефа между проходами имеет эффект "золотой середины", когда возникает эффект асимметрии, но разница в значениях деформации не так велика, как в предыдущем случае. Реализация этой схемы потребует визуального или автоматического контроля величины сдвига на период рельефа путем изменения конфигурации направляющих линеек.

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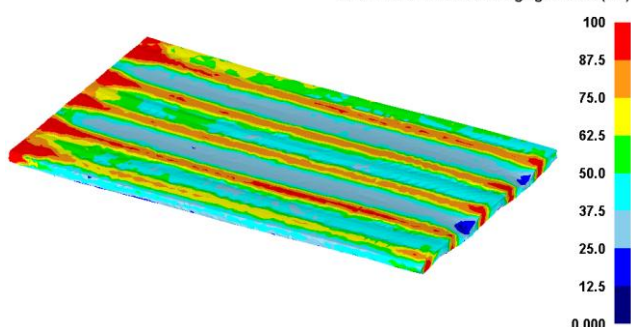
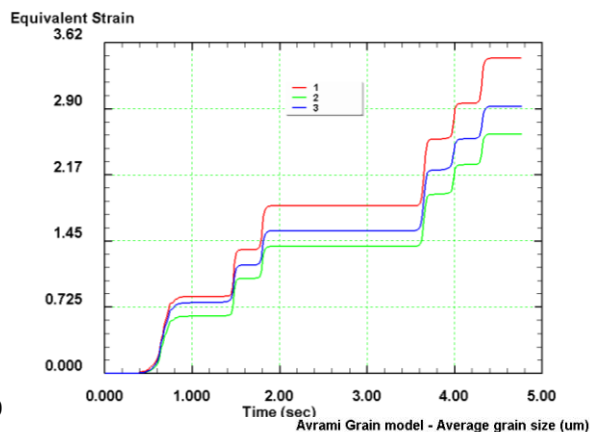


Рис. 3. Эквивалентная деформация (а) и эволюция микроструктуры (б) после двух проходов без изменения положения заготовки

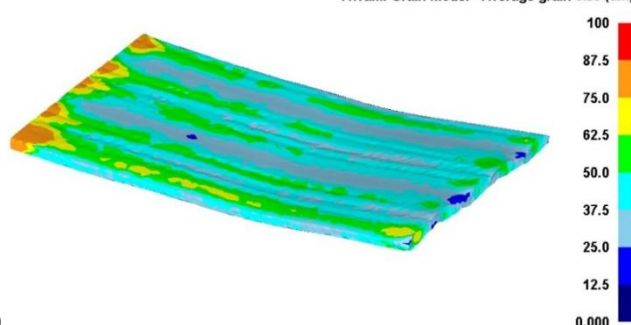
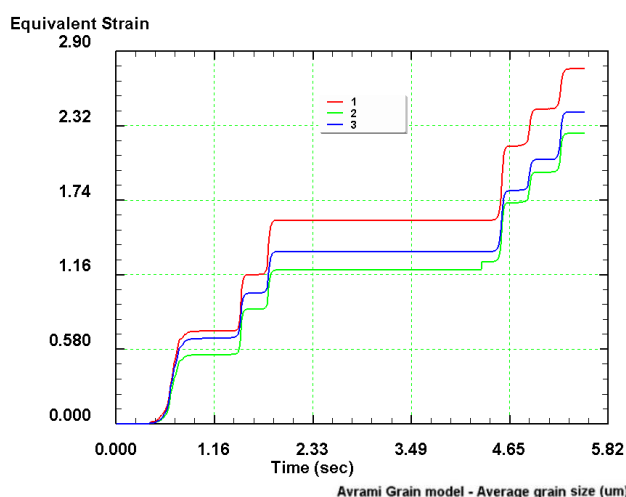


Рис. 4. Эквивалентная деформация (а) и эволюция микроструктуры (б) после двух проходов с поперечным смещением заготовки за период рельефа

Isentropic and exergy analyses of turbomachines from CO₂ supercritical power plant

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Abstract: The results of three turbomachines (one turbocompressor and two turbines) isentropic and exergy analyses, which operate in supercritical CO₂ power plant are presented in this paper. Both observed turbines (Turbine 1 and Turbine 2) have higher improvement potential than Turbocompressor. Mechanical losses in power transmission between Turbine 1 and Turbocompressor are equal to 456.57 kW in real operation process. Turbocompressor has the highest isentropic efficiency of 96.87% and the highest exergy efficiency of 97.61% if all observed turbomachines are considered. Turbine 2 used for the electric generator drive has higher efficiencies (both isentropic and exergy) in comparison to Turbine 1, regardless of higher isentropic loss and higher exergy destruction. Increase in the ambient temperature from 5 °C up to 45 °C decreases Turbocompressor exergy efficiency for 0.31%, while the same ambient temperature increase decreases exergy efficiency of both turbines for 0.53% (Turbine 1) and for 0.52% (Turbine 2).

KEYWORDS: TURBOMACHINES, ISENTROPIC ANALYSIS, EXERGY ANALYSIS, CO₂, SUPERCRITICAL POWER PLANT

1. Introduction

Open-cycle gas turbine power plants have nowadays various applications in the energy sector (as independent plants, or in a combination with some other mechanical power producers) [1, 2]. Closed-cycle gas turbine power plants are not widely distributed as open-cycle gas turbine power plants, but they may have some interesting applications [3, 4]. In recent years, closed-cycle gas turbine power plants in various arrangements are often used as waste heat recovery systems in marine sector [5, 6].

It is well known from the literature that closed-cycle gas turbine power plants efficiency change is much lower at partial loads in comparison to open-cycle gas turbine power plants, what is one of their notable benefits [7]. Moreover, the produced mechanical power in closed-cycle gas turbine power plants can be easily regulated by changing operating fluid mass flow rate [8]. However, closed-cycle gas turbine power plants are usually much more complex in comparison to open-cycle gas turbine power plants, operating fluids used in closed-cycle gas turbine power plants are expensive and they are not always available in the market, etc., so it is obvious that closed-cycle gas turbine power plants also have some disadvantages in comparison to open-cycle gas turbine power plants.

In this paper are analyzed three turbomachines (one turbocompressor and two turbines) which operate in supercritical CO₂ power plant from the isentropic and exergy viewpoint. Efficiencies and losses (destructions) of all turbomachines are compared and the guidelines for possible improvements are presented. Moreover, it is performed analysis related to the ambient temperature change influence on each turbomachine exergy efficiency and destruction.

2. Description of the analyzed CO₂ supercritical power plant and its turbomachines

General scheme of the CO₂ supercritical power plant in which operates turbocompressor and both turbines analyzed in this paper is presented in Fig. 1.

CO₂ with the lowest temperature in the process enters in the Turbocompressor (operating point 1, Fig. 1). Turbocompressor increases CO₂ pressure (and simultaneously CO₂ temperature) and delivers it to the recuperator (operating point 2, Fig. 1). Recuperator is a counter flow CO₂-CO₂ heat exchanger in which CO₂ after the expansion in Turbine 2 (operating point 6, Fig. 1) is used for heating the lower temperature CO₂ which enters in the recuperator from Turbocompressor. CO₂ with an increased temperature from the recuperator (operating point 3, Fig. 1) enters in the main heater which increases CO₂ temperature at the highest possible level in the plant (operating point 4, Fig. 1). After the main heater, CO₂ expands through Turbine 1 (the only task of Turbine 1 is mechanical power production for the Turbocompressor drive). From the Turbine 1 outlet (operating point 5, Fig. 1), CO₂ is delivered directly to the Turbine 2 inlet through which expands. Turbine 2 is used in this

power plant for the electric generator drive and therefore for the electricity production. After the expansion in Turbine 2, CO₂ is sent to recuperator (operating point 6, Fig. 1) inside which it transfers heat to colder CO₂. After heat transfer in recuperator (operating point 7, Fig. 1), CO₂ is sent to the main cooler inside which is cooled to the lowest possible temperature in the observed process (operating point 1, Fig. 1). For the cooling purposes in the main cooler can be used various fluids (however, the most used cooling fluid is water).

For the power plant presented in Fig. 1 are analyzed in this paper only the turbomachines because some fluid flow streams and their operating parameters for several heat exchangers are unknown, so the proper energy and exergy analyses cannot be performed for these components. For example, for the main heater are unknown operating parameters of the heating fluid at the main heater inlet and outlet as well as operating parameters of the cooling fluid at the main cooler inlet and outlet, so the proper energy and exergy analyses cannot be performed for these power plant components.

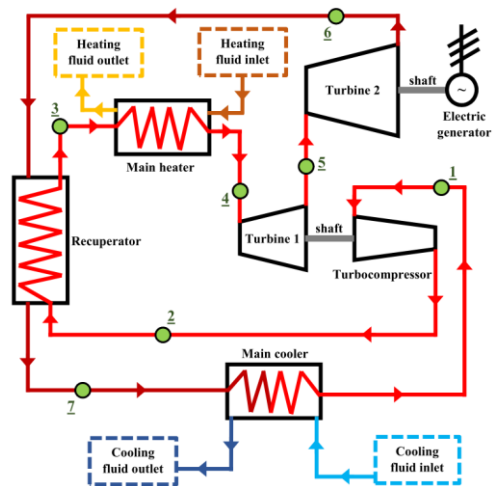


Fig. 1. General scheme of the supercritical CO₂ power plant and operating points required for the turbomachines (Turbocompressor, Turbine 1 and Turbine 2) isentropic and exergy analyses

Isentropic analysis of any turbomachine is a comparison of ideal (isentropic) and real (polytropic) compression or expansion process. Data of real (polytropic) compression or expansion processes are obtained from the measurements during the plant exploitation, while the data of ideal (isentropic) processes are obtained by mathematical calculations. Ideal (isentropic) process is the process between the same pressures and it uses the same mass flow rates as the real (polytropic) process, but in ideal process fluid (in this case CO₂) specific entropy remains constant, Fig. 2 [9]. For the observed turbocompressor and both turbines operating point at the end of ideal (isentropic) process is obtained by knowing fluid pressure at the end of the process and fluid specific entropy which remains the same as at the process beginning, Fig. 2. Ideal (isentropic)

compression or expansion process did not consider any losses, losses are considered in the real (polytropic) processes and they are proportional to the increase in fluid specific entropy.

The difference between turbocompressor and any turbine is that turbocompressor is the mechanical power consumer – in an ideal (isentropic) compression process turbocompressor will consume the lowest possible mechanical power, while in real (polytropic) compression process, due to losses occurrence, turbocompressor will consume higher mechanical power in comparison to ideal process. Turbine is a mechanical power producer – in an ideal (isentropic) expansion process turbine will produce the highest possible mechanical power, while in real (polytropic) expansion process, due to losses occurrence, turbine will produce lower mechanical power in comparison to ideal process. These considerations related to ideal and real compression and expansion processes are valid for any mechanical power consumer and producer, not only for the turbocompressor and turbines analyzed in this paper.

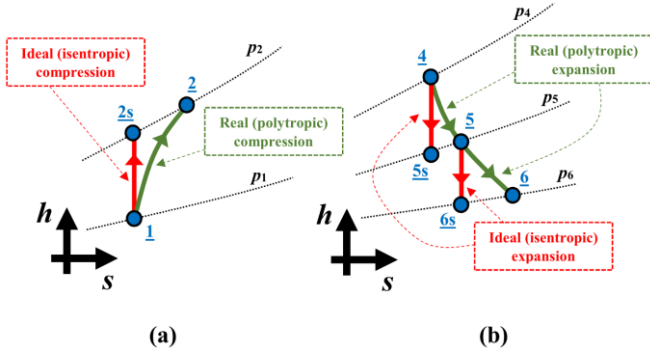


Fig. 2. Comparison of ideal and real compression and expansion processes: (a) Turbocompressor; (b) Turbine 1 and Turbine 2

3. Turbomachines analyses equations and principles

Isentropic and exergy analyses of all turbomachines from the observed CO₂ supercritical power plant are performed according to guidelines, recommendations and equations from the available literature [10-12]. Due to the limited space, baseline equations related to any turbomachine isentropic and exergy analyses are not presented in this paper, but they can be found in [13, 14].

The main difference between isentropic and exergy analyses of any turbomachine is that in the isentropic analysis are not considered the parameters of the ambient (ambient pressure and temperature) inside which turbomachine operate (turbomachine isentropic analysis is a comparison of ideal and real operating process), while exergy analysis considers the ambient parameters [7, 15]. Therefore, in exergy analysis can be investigated the influence of the ambient parameters change on the turbomachine (or any other component) operating characteristics [16, 17].

Isentropic and exergy analysis equations of each observed turbomachine are defined in accordance with operating points presented in Fig. 1 and Fig. 2. Exergy analysis equations of each turbomachine remain the same, regardless of the selected ambient parameters.

3.1. Turbomachines isentropic analysis equations

TURBOCOMPRESSOR

Consumed real (polytropic) mechanical power:

$$P_{re,TC} = \dot{m}_1 \cdot (h_2 - h_1), \quad (1)$$

where P is mechanical power, $\dot{m}$ is CO₂ mass flow rate and h is CO₂ specific enthalpy. Mechanical power which will be consumed in an ideal situation is:

$$P_{id,TC} = \dot{m}_1 \cdot (h_{2s} - h_1). \quad (2)$$

Turbocompressor isentropic loss is:

$$IS_{loss,TC} = P_{re,TC} - P_{id,TC}, \quad (3)$$

while Turbocompressor isentropic efficiency is:

$$\eta_{IS,TC} = \frac{P_{id,TC}}{P_{re,TC}}. \quad (4)$$

TURBINE 1

Produced real (polytropic) mechanical power:

$$P_{re,TURB1} = \dot{m}_4 \cdot (h_4 - h_5). \quad (5)$$

Ideal (isentropic) mechanical power is:

$$P_{id,TURB1} = \dot{m}_4 \cdot (h_4 - h_{5s}). \quad (6)$$

Turbine 1 isentropic loss is:

$$IS_{loss,TURB1} = P_{id,TURB1} - P_{re,TURB1}, \quad (7)$$

while Turbine 1 isentropic efficiency is:

$$\eta_{IS,TURB1} = \frac{P_{re,TURB1}}{P_{id,TURB1}}. \quad (8)$$

TURBINE 2

Produced real (polytropic) mechanical power:

$$P_{re,TURB2} = \dot{m}_5 \cdot (h_5 - h_6). \quad (9)$$

Ideal (isentropic) mechanical power:

$$P_{id,TURB2} = \dot{m}_5 \cdot (h_5 - h_{6s}). \quad (10)$$

Turbine 2 isentropic loss is:

$$IS_{loss,TURB2} = P_{id,TURB2} - P_{re,TURB2}, \quad (11)$$

while Turbine 2 isentropic efficiency is:

$$\eta_{IS,TURB2} = \frac{P_{re,TURB2}}{P_{id,TURB2}}. \quad (12)$$

3.2. Turbomachines exergy analysis equations

Exergy analysis of any observed turbomachine considers real (polytropic) compression and expansion processes only as well as fluid (CO₂) total exergy flows.

TURBOCOMPRESSOR

Turbocompressor cumulative exergy inlet is:

$$\dot{E}x_{inlet,TC} = \dot{m}_1 \cdot \varepsilon_1 + P_{re,TC}, \quad (13)$$

where $\dot{E}x$ is fluid total exergy flow and ε is fluid specific exergy.

Turbocompressor cumulative exergy outlet is:

$$\dot{E}x_{outlet,TC} = \dot{m}_2 \cdot \varepsilon_2, \quad (14)$$

while Turbocompressor exergy destruction is:

$$\dot{E}x_{destruction,TC} = \dot{E}x_{inlet,TC} - \dot{E}x_{outlet,TC}. \quad (15)$$

Turbocompressor exergy efficiency is:

$$\eta_{EX,TC} = \frac{\dot{m}_2 \cdot \varepsilon_2 - \dot{m}_1 \cdot \varepsilon_1}{P_{re,TC}}. \quad (16)$$

TURBINE 1

Turbine 1 cumulative exergy inlet is:

$$\dot{E}x_{inlet,TURB1} = \dot{m}_4 \cdot \varepsilon_4. \quad (17)$$

Turbine 1 cumulative exergy outlet is:

$$\dot{E}x_{outlet,TURB1} = \dot{m}_5 \cdot \varepsilon_5 + P_{re,TURB1}, \quad (18)$$

while Turbine 1 exergy destruction is:

$$\dot{E}x_{destruction,TURB1} = \dot{E}x_{inlet,TURB1} - \dot{E}x_{outlet,TURB1}. \quad (19)$$

Turbine 1 exergy efficiency is:

$$\eta_{EX,TURB1} = \frac{P_{re,TURB1}}{\dot{m}_4 \cdot \varepsilon_4 - \dot{m}_5 \cdot \varepsilon_5}. \quad (20)$$

TURBINE 2

Turbine 2 cumulative exergy inlet is:

$$\dot{E}x_{\text{inlet,TURB2}} = \dot{m}_5 \cdot \varepsilon_5 \quad (21)$$

Turbine 2 cumulative exergy outlet is:

$$\dot{E}x_{\text{outlet,TURB2}} = \dot{m}_6 \cdot \varepsilon_6 + P_{\text{re,TURB2}} \quad (22)$$

while Turbine 2 exergy destruction is:

$$\dot{E}x_{\text{destruction,TURB2}} = \dot{E}x_{\text{inlet,TURB2}} - \dot{E}x_{\text{outlet,TURB2}} \quad (23)$$

Turbine 2 exergy efficiency is:

$$\eta_{\text{EX,TURB2}} = \frac{P_{\text{re,TURB2}}}{\dot{m}_5 \cdot \varepsilon_5 - \dot{m}_6 \cdot \varepsilon_6} \quad (24)$$

4. CO₂ operating parameters required for the turbomachines isentropic and exergy analyses

CO₂ operating parameters (temperatures and pressures) in each operating point from Fig. 1 are found in the literature [18] and presented in Table 1. It should be highlighted that CO₂ mass flow rate selected in this paper is notably higher than proposed in [18]. Other operating parameters presented in Table 1 which are not found in the literature are calculated by using NIST-REFPROP 9.0 software [19].

In exergy analysis of any system or component a definition of the base ambient state is required [20, 21]. In this paper, the base ambient state is defined by the ambient temperature of 25 °C and the ambient pressure of 1 bar.

CO₂ operating parameters in operating points from Fig. 2 related to ideal (isentropic) compression and expansion processes are presented in Table 2.

Table 1. CO₂ operating parameters in each operating point from Fig. 1 – real (polytropic) compression and expansion processes

O. P. *	Temp. (°C)	Pressure (bar)	Mass flow rate (kg/s)	Specific enthalpy (kJ/kg)	Specific entropy (kJ/kg·K)	Specific exergy (kJ/kg) **
1	65.56	105.49	57	431.49	1.7182	230.10
2	126.56	233.04		466.58	1.7210	264.35
3	582.61	229.60		1073.90	2.7602	561.85
4	732.22	227.53		1263.40	2.9660	689.97
5	696.94	176.67		1220.30	2.9723	644.97
6	637.50	113.76		1149.10	2.9821	570.81
7	132.06	106.81		545.01	2.0256	251.97

* O. P. = Operating Point (in accordance to Fig. 1)

** At the base ambient state (25 °C, 1 bar)

Table 2. CO₂ operating parameters in operating points from Fig. 2 – ideal (isentropic) compression and expansion processes

O. P.*	Pressure (bar)	Mass flow rate (kg/s)	Isentropic specific enthalpy (kJ/kg)	Specific entropy (kJ/kg·K)
1	105.49	57	431.49	1.7182
2s	233.04		465.48	1.7182
4	227.53		1263.40	2.9660
5s	176.67		1214.20	2.9660
5	176.67		1220.30	2.9723
6s	113.76		1140.10	2.9723
7	106.81		545.01	2.0256

* O. P. = Operating Point (in accordance to Fig. 2)

5. Results and discussion

Real and ideal mechanical power (consumed by the turbocompressor and produced by the turbines) is presented in Fig. 3. In an ideal (isentropic) compression process Turbocompressor consumes lower mechanical power than in the real (polytropic) process (1937.43 kW in comparison to 2000.13 kW), because Turbocompressor is mechanical power consumer. Each turbine in ideal (isentropic) expansion process produces higher mechanical

power than in real (polytropic) expansion process because turbine is a mechanical power producer (ideal and real mechanical power produced in Turbine 1 are 2804.40 kW and 2456.70 kW, while in Turbine 2 are 4571.40 kW and 4058.40 kW), Fig. 3. Ideal mechanical power consumed by Turbocompressor and produced in each turbine shows the best possible option, and these results can be used as the guideline for the improvements and losses reduction.

In the observed process, Fig. 1, mechanical power produced in the Turbine 1 is used for the Turbocompressor drive only. Therefore, in real (polytropic) process, Turbine 1 produces slightly higher mechanical power than is consumed by Turbocompressor, which means that mechanical losses in power transmission (real process) from Turbine 1 to Turbocompressor are equal to 456.57 kW.

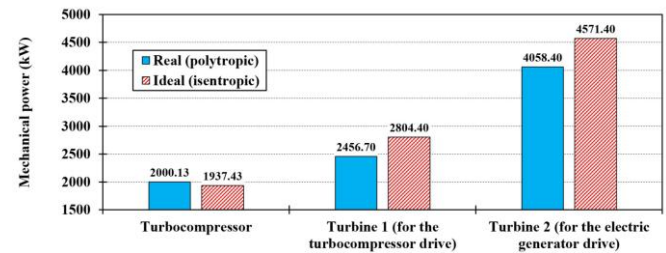


Fig. 3. Real and ideal mechanical power (consumed by the turbocompressor and produced by the turbines)

Isentropic and exergy analysis results of each observed turbomachine are presented in Fig. 4 and Fig. 5. From Fig. 4 and Fig. 5 is clear that both isentropic and exergy analyses show the same trends and general conclusions.

The lowest isentropic loss and the lowest exergy destruction of all observed turbomachines has Turbocompressor – consequentially, Turbocompressor has the highest isentropic efficiency of 96.87% and the highest exergy efficiency of 97.61% if all observed turbomachines are considered. Regardless of the fact that Turbine 2 used for the electric generator drive has higher isentropic loss and higher exergy destruction in comparison to Turbine 1, Turbine 2 has higher efficiencies (both isentropic and exergy) in comparison to Turbine 1. Turbine 2 isentropic efficiency is 88.78%, while its exergy efficiency is 96.01%.

In similar closed-cycle gas turbine power systems from the literature [5, 7] can be seen that efficiencies of the turbines (both isentropic and exergy) are higher in comparison to turbocompressors, while for the turbomachines from closed-cycle gas turbine power plant analyzed in this paper is obtained reverse conclusion. The reason for such occurrence can be found in the presented CO₂ operating parameters (Table 1) which seems to be optimal for the Turbocompressor and not fully optimal for Turbine 1 and Turbine 2.

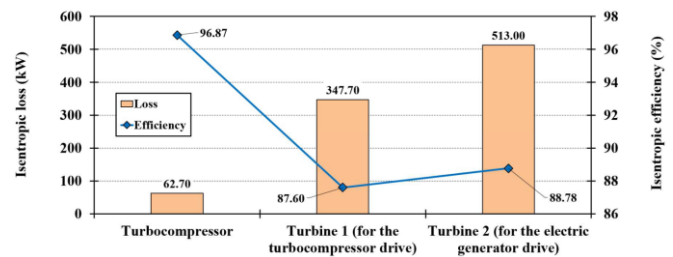


Fig. 4. Isentropic loss and isentropic efficiency of turbocompressor and both turbines

The last part of this research involves analysis related to the exergy parameters sensitivity to the ambient temperature change of all observed turbomachines. Exergy parameters sensitivity is investigated in the ambient temperature range from 5 °C up to 45 °C, while the ambient pressure remains the same as at the base ambient state (1 bar). For all analyzed turbomachines is valid a conclusion that increase in the ambient temperature simultaneously increases exergy destructions and decreases exergy efficiencies,

what is also valid for many other components from various power systems [13, 14]. Turbocompressor is the least sensitive to the ambient temperature change of all observed turbomachines, while the sensitivity of both turbines is very similar. Increase in the ambient temperature from 5 °C up to 45 °C decreases Turbocompressor exergy efficiency for 0.31%, while the same ambient temperature increase decreases exergy efficiency of both turbines for 0.53% (Turbine 1) and for 0.52% (Turbine 2). Finally, it can be concluded as in [22, 23] that exergy parameters of turbomachines in general are not highly influenced by the ambient temperature change.

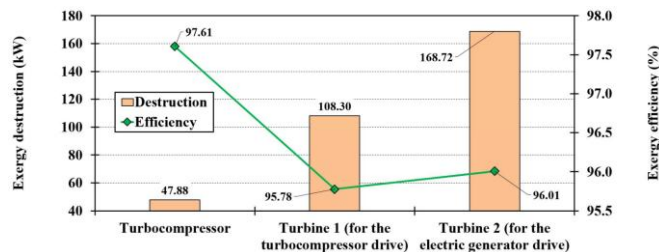


Fig. 5. Exergy destruction and exergy efficiency of turbocompressor and both turbines at the base ambient state

6. Conclusions

In this paper are presented results of three turbomachines (one turbocompressor and two turbines) isentropic and exergy analyses. Analyzed turbomachines operate in supercritical CO₂ power plant. The most important obtained conclusions are:

- Both observed turbines (Turbine 1 and Turbine 2) have higher improvement potential than Turbocompressor due to the higher difference between ideal and real mechanical power.
- Mechanical losses in power transmission between Turbine 1 and Turbocompressor are equal to 456.57 kW in real operation process.
- Turbocompressor has the highest isentropic efficiency of 96.87% and the highest exergy efficiency of 97.61% if all observed turbomachines are considered.
- Regardless of the fact that Turbine 2 used for the electric generator drive has higher isentropic loss and higher exergy destruction in comparison to Turbine 1, Turbine 2 has higher efficiencies (both isentropic and exergy) in comparison to Turbine 1. Turbine 2 isentropic efficiency is 88.78%, while its exergy efficiency is 96.01%.
- Increase in the ambient temperature from 5 °C up to 45 °C decreases Turbocompressor exergy efficiency for 0.31%, while the same ambient temperature increase decreases exergy efficiency of both turbines for 0.53% (Turbine 1) and for 0.52% (Turbine 2).
- In general, exergy parameters of turbomachines are not notably influenced by the ambient temperature change.

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The solution of the boundary value problems of the transfer processes in multilayer enclosing structures

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Abstract: By means of generalized functions analytical closed solutions of non-stationary transfer in multilayer enclosing structures of canonical forms under asymmetric boundary conditions of the first, second, third and mixed kinds were obtained.

KEY WORDS: MODELING, SOLUTION, MULTILAYER STRUCTURE, UNIT FUNCTION, THERMOPHYSICAL CHARACTERISTICS.

1. Introduction

The processes of heat and mass transfer and filtration of liquids and vapour-gas mixtures through the capillaries of multilayer enclosing structures are very complex and closely interconnected. In addition, depending on the period of the year, they are accompanied by physically related phenomena such as infiltration and exfiltration of ambient air; evaporative cooling or condensation heating. The implementation of the dense outer layer of the enclosing structures of buildings and structures is not possible in all cases, because such a constructive solution worsens the moisture condition of the enclosure due to difficulties in air permeability and, consequently, and its drying in the summer season [1,2].

Modern multilayer energy-saving enclosing structures (which in a broad sense, in addition to the enclosing structures, they also mean thermal, engineering and electrical networks, "clothing" of roads, tanks and reservoirs for heating, cooling or storing any liquids or gases, etc.) mainly consist of capillary-porous material, which are increasingly used not only in construction, but also in many other industries (high-temperature heat exchangers, turbine blades, rocket nozzles, cladding of high-speed flying machines, cladding of heat and power generating units, systems of nuclear reactors with internal cooling, etc.), where various elements of equipment where various items of equipment are subject to sufficiently high thermal stresses and pressures resulting from large gradients of transfer potentials (temperature, pressure and mass content) [3-9].

2. Main Body

In the most general case the nonlinear differential equation system of convective non-stationary transfer can be written in the vector-matrix form:

$$D\bar{S}[\bar{\Pi}(\bar{x}, \tau)] + \bar{\tau}_r \bar{S}_{\tau\tau}[\bar{\Pi}(\bar{x}, \tau)] + \text{sgn}[\bar{J}] < \bar{\nabla}, \bar{J}[\bar{\Pi}(\bar{x}, \tau)] > + \text{sgn}[\bar{I}] [\bar{\Pi}(\bar{x}, \tau)] = \bar{0} \quad ((1))$$

The system (1) also describes high-intensity, high-speed and high-temperature processes (second member of the equation), when the speed of propagation of the substance is comparable with the speed of the processes themselves (metal cutting, laser welding, etc.), i.e., when both the relaxation time of the densities of the flows of substances and the time of their damping $\nabla \bar{\Pi}(\bar{x}, \tau)$ can be taken into account. If to be based on the phenomenological theory of the transfer processes, then there will be no second member of the nonlinear differential equation system (1), because the propagation speed of the flows of substances tends to infinity, and $\bar{\tau}_r$ tends to zero [3,10]. In this case, the nonlinear differential equation system (1) comes over from the hyperbolic type to the parabolic type, which describes the irreversible processes of convective conjugate transfer and, in particular, heat and mass transfer processes.

Particularly posed are boundary-value problems when differential equations (DEs) are equations of mixed type, i.e. when in different parts of the considered region of independent variable multilayer construction the differential operator (D) belongs to different (hyperbolic, parabolic and elliptical) types [11,12], i.e. when $\nabla \bar{\Pi}(\bar{x}, \tau)$ in separate layers of multilayer construction differ from each other by significant values.

High-intensity technological processes of heat and mass transfer in modern technology now have a non-stationary nonlinear character, because at sufficiently high concentrations (temperatures), the heat and mass transfer coefficients depend on the potentials themselves $[K(\bar{\Pi})]$, then the corresponding nonlinear differential equation system (or nonlinear transfer equation) is solved only numerically or approximately by special methods [11-18, 22-28, 38, 44, 54]. For such transfer processes the nonlinear differential equation system in heterogeneous bodies of arbitrary geometric shape is reduced to the integration of the following system, presented in the vector-matrix notation:

$$D\bar{\Pi} + \sum_{i=2}^n \tau_j^{i-1} \bar{\Pi}^{(i)} = \text{sgn}[\bar{J}] \sum_{i=1}^m \tau_{\bar{\Pi}}^{i-1} < \bar{\nabla}, [K(\bar{\Pi})][\bar{\nabla} \bar{\Pi}]^{(i-1)} > + \text{sgn}[\bar{I}] \sum_{i=1}^n \tau_j^{i-1} \bar{I}^{(i-1)} \quad (2)$$

or in the scalar notation

$$D\Pi_i + \sum_{i=2}^n \tau_{j_i}^{i-1} \Pi_i^{(i)} = \text{sgn}[\bar{J}_i] \sum_{i=1}^m \tau_{\bar{\Pi}_i}^{i-1} < \bar{\nabla}, [k_{ij}(\Pi_j)][\bar{\nabla} \Pi_j]^{i-1} > + \text{sgn}[\bar{I}_i] \sum_{i=1}^n \tau_{j_i}^{i-1} \bar{I}^{(i-1)}, \quad i = \overline{1, n} \quad (3)$$

With a constant matrix of coefficients of the nonlinear differential equation system (2) and (3) can be rewritten, accordingly, in the form:

$$D\bar{\Pi} + \sum_{i=2}^n \tau_j^{i-1} \bar{\Pi}^{(i)} = \text{sgn}[\bar{J}] \sum_{i=1}^m \tau_{\bar{\Pi}}^{(i-1)} [K][\bar{\nabla}^2 \bar{\Pi}]^{i-1} + \text{sgn}[\bar{I}] \sum_{i=1}^n \tau_j^{i-1} \bar{I}^{(i-1)}, \quad (4)$$

$$D\Pi_i + \sum_{i=2}^n \tau_{j_i}^{i-1} \Pi_i^{(i)} = \text{sgn}[\bar{J}_i] \sum_{i=1}^m \tau_{\bar{\Pi}_i}^{i-1} \sum_{j=1}^n k_{ij} \nabla^2 \Pi_j^{(i-1)} + \text{sgn}[\bar{I}_i] \sum_{i=1}^n \tau_{j_i}^{i-1} \bar{I}_i^{(i-1)}, \quad i = \overline{1, n}. \quad (5)$$

In the absence of convective transfer, the nonlinear differential equation system (2) can be rewritten in the form:

$$\sum_{i=1}^n \tau_j^{i-1} \bar{\Pi}^{(i)} = \text{sgn}[\bar{J}] \text{div} \sum_{i=1}^m [K][\tau_{\bar{\Pi}}^{i-1} \bar{\nabla} \bar{\Pi}^{(i-1)}] + \text{sgn}[\bar{I}] \sum_{i=1}^n \tau_j^{i-1} \bar{I}^{(i-1)}. \quad (6)$$

From (6), the nonlinear differential equation system of the inter-related and unrelated transfer by hypotheses follows:

- 1- Fourier (for $n = 1$ and $m = 1$), when there are no time derivatives of flows of substances and gradients of transport potentials (DE of parabolic type);
 - 2- Cattaneo Vernotte (for $n=2, m=1$), taking into account the first time derivatives of the flows of transferred substances $\frac{\partial \bar{J}(\bar{x}, \tau)}{\partial \tau}$ (DU of hyperbolic type);
 - 3- Maxwell – Cattaneo - Lykov (for $n=2$ and $m= 2$), taking into account the first derivatives of the flows and gradients of the potentials of substances $\frac{\partial \bar{J}(\bar{x}, \tau)}{\partial \tau}$ and $\frac{\partial \nabla \bar{\Pi}(\bar{x}, \tau)}{\partial \tau}$ (DU of hyperbolic type);
 - 4- The nonlinear differential equation system and DE (for $n \geq 3$ and $m \geq 3$), taking into account the second derivatives and higher in time by flows and gradients of transport potentials.
- The physical justification for the need to take into account derivatives of a higher order is still not enough weight. Therefore, the adequacy of their accounting requires additional resolution using experimental-theoretical research. In addition, the appearance of additional terms in the nonlinear differential equation system and DE noticeably complicates the calculations of transient transfer processes [29–37, 39–52, 56].

If it is necessary to take into account the convective transfer, the convective component of the Lagrange derivative is added to the first term of the left-hand side of the nonlinear differential equation system(6). For example, according to the Fourier hypothesis, the nonlinear differential equation system of the heat and mass transfer in scalar form at $[k_{ij}] = \text{var}$, will be:

$$D\Pi_i = \text{sgn}[\bar{J}_i] < \nabla, \sum_{j=1}^n k_{i,j} (\Pi_j) \nabla \Pi_j > + \text{sgn}[I_i] I_i(\bar{x}, \tau);$$

$$i = \overline{1, n},$$

$$\text{for } [k_{ij}] = \text{const} \quad (7)$$

$$D\Pi_i = \text{sgn}[\bar{J}_i] \sum_{j=1}^n k_{i,j} \nabla^2 \Pi_j + \text{sgn}[I_i] I_i(\bar{x}, \tau), \quad i = \overline{1, n}. \quad (8)$$

When setting the boundary-value problem (according to the Fourier hypothesis) in heterogeneous media, the matrix of transfer coefficients $[K]$ mainly depends only on the spatial coordinates $\bar{x}$, but because the nonlinear differential equation system (or equation) of transfer includes the second derivatives of the required transfer potentials by variable $\bar{x}$, then it can no longer be reduced to the differential equation system with constant coefficients and it must be solved only by approximate methods. For example, for engineering calculations, approximate analytical methods for solving the boundary-value problem are widely used. These are variational methods (Ritz, Trefftz, A.V. Kantorovich and others); methods of weighted residuals (Bubnov-Galerkin orthogonal method, collocations, moments, least squares, etc.); operational methods (Laplace, infinite and finite Fourier transforms, Hankel, etc.); integral methods of heat balance, averaging of functional corrections, methods of M. Bio, M.E. Shvets, A.I. Veinik and others, in which the model of potential disturbance is used (for example, the penetration depth of the thermal layer); methods for sharing accurate (separation of variables, integral transforms, thermal potentials, etc.) and the above approximate analytical methods [12-18, 28, 33, 36, 38].

One of the simple methods for an approximate solution is to replace $[K(\bar{x})]$ by piecewise constant functions. For this, the intervals of change of $\bar{x}$ (all axes, semi-axes, or finite intervals) are divided into partial intervals $(\bar{x}_{i-1}, \bar{x}_i)$ and in each partial interval are considered $[K] = [K_i(\bar{x}_i)]$ constant for $\forall \bar{x}_i \in (\bar{x}_{i-1}, \bar{x}_i)$, and then the posed boundary-value problem is already solved by known methods [11–13, 18, 24, 26, 54, 55] with the boundary conditions for “gluing” the solution. If $\bar{x}_i$ – is the division point (boundary or surface) of two adjacent partial intervals, then the transfer potentials $\bar{\Pi}(\bar{x}_i)$ in it are assumed to be continuous or the middle of the jumps of the functions $\bar{\Pi}(\bar{x}_i)$ at the points of a removable discontinuity $\bar{x}_i$ of the first kind (for example, when contact thermal resistance of two adjacent of multilayer construction layers is taken into account).

Somewhat simpler, but practically important, are the transfer processes passing through a finite number of layers, i.e. through a piecewise homogeneous medium. The mathematical formulation of the such boundary-value problem can be written in the form:

$$\frac{\partial \Pi_i}{\partial \tau} = k_i \Delta \Pi_i + I_i(\bar{x}, \tau), \quad i = \overline{1, n}, \quad (9)$$

where the transfer potential $\Pi_i(\bar{x}, \tau)$ means either the mass transfer potential (moisture content, substance concentration) or temperature, and k_i means the constants, respectively, either the diffusion coefficient or thermal diffusivity of the i -th layer of the multilayer construction.

The differential equation system of interconnected heat and mass transfer for piecewise homogeneous media under a number of simplifying assumptions (when $Bi_m > 100$, and $Lu \gg 1$ or $Lu \ll 1$) and the condition of the zonal method of calculation (or application of the local coordinate system), when the transfer coefficients are accepted independent of coordinates, are also reduced to consideration the differential equation system of unrelated transfer (9) [4]. The solution of such problems under various single-valued conditions can be found in [4, 14, 15, 25] and other sources.

For a generalized analytical solution by the Fourier method of similar linear boundary-value problems (parabolic, hyperbolic and elliptic types) with linear additional conditions (for example, when a linear combination of $\Pi(\bar{x}, \tau)$ and its normal derivative is given on the surface (or contour) of the region) are preliminarily reduced to the simpler boundary-value problems, then their general solution is obtained from the superposition principle. The limiting problems of transfer processes are also solved in a same way.

It should be noted that when setting such boundary-value problems, due to the definiteness and continuity of $\bar{\Pi}(\bar{x}, \tau)$ in the closed (considered) region and $\bar{\Pi}(\bar{x}, \tau)$ satisfies the transfer equations in the open region, the continuity of the initial and boundary conditions and the requirement of their compatibility with each other follow. However, the conditions for the continuity of the initial value and the conditions for its conjugation with the boundary values are very restrictive and often exclude practically important cases from consideration. In these cases, the boundary-value problems are considered with piecewise continuous initial functions, not assuming that the initial function is associated with boundary conditions or the filtering property of the Dirac impulse function is used to construct the influence function (Green), which allows to find an integral solution of the heterogeneous DE satisfying homogeneous boundary conditions. To solve non-stationary boundary-value transfer problems in multilayer constructions, the mathematical theory of generalized functions is successfully used (the delta-Dirac function and its filtering property; Heaviside unit function, asymmetric unit function, other step functions), which allows one to adequately describe the distributions of different discontinuous physical characteristics of a piecewise homogeneous medium and in closed form to obtain analytical solutions of boundary-value problems by reducing multilayer constructions to single-layer ones [4,13-17].

In many important applied boundary-value problems of molecular diffusion and thermal conductivity for piecewise homogeneous media, one has to deal with boundary conditions, when the concentration (temperature) of the substance at the boundary of the layer is actually some given function of time (i.e. it is the solution of the boundary-value problem for the previous layer at its given thickness) and this value, due to the “gluing” condition, serves as the boundary condition for concentration (temperature) on the segment of the next homogeneous layer [11,12,18]. An analytical solution to such non-stationary boundary-value problem is applied for mathematical modeling (MM) of desalination of drinking water at the ultrafiltration nanomembrane combined water treatment plant for water and heat supply systems. An MM of the process of filtering a crude liquid with a given constant concentration of suspended colloidal particles, diffusion coefficient and fluid flow through the adsorbent layer, which contains a medium with its diffusion coefficient. From some initial moment of

time the diffusion process begins, during which it is necessary to determine the change in the concentration of suspended and colloidal particles in a given region of the event space (independent variables).

In a stationary formulation for non-linear heat transfer taking into account filtration (gas, steam-gas mixture, liquid) and the presence of internal volumetric drains (moisture) or heat sources under generally accepted assumptions [1,2] in the one-dimensional case as applied to canonical forms in the corresponding coordinate systems, the system (1) the system can be written in the form of an ordinary differential heterogeneous second-order equation [19-21].

In the physical description of the cooling processes of the enclosing structure (possibly evaporative) or heating (possibly condensation), thermal balances can be compiled similarly to equation (1) both for the region $r \in [-\infty, 0]$, and for the region $r \in [h, +\infty]$, which lead to new DEs of gas (or liquid) flows running towards the enclosing structure and moving away from the enclosing structure with boundary conditions corresponding to new closed intervals r . In this case, one or two second-order DEs and, accordingly, two or four boundary conditions are added to the nonlinear differential equation system (1) depending on the conditions of the problem. By this means, the generalized MM, even for stationary heat transfer in the building envelope, must contain three second-order DEs and six boundary conditions for finding the corresponding integration constants. In this case, the temperature field $T(r)$ in the enclosing structure expressed through the ambient air temperatures (gas, liquid, coolant or refrigerant) on both sides. In a more simplified version, these boundary DEs for the enclosing structure are replaced by boundary conditions of the third kind, with possible consideration of surface runoff or heat sources at the boundary of the enclosing structure surfaces [3,22,23]. Conversely, equation (1) with boundary conditions of the third kind can be replaced by simpler boundary conditions of the first kind provided that constant fictitious (equivalent) boundary layers are introduced. An analysis of convective heat transfer shows that in this case the boundary conditions of the third kind are actually displayed in the boundary conditions of the first kind. Then, when integrating the DE (1) and the presence of two isothermal surfaces in boundary conditions, we can use the Kirchhoff transformation [22, 23], which through a new auxiliary variable and the average coefficient of thermal conductivity leads DE (1) to formalize the first boundary-value problem.

A boundary-value problem formalized in this way can be written through the Peclet criteria (Pe), Pomerantsev criteria (Po), dimensionless scales of temperature and thermal resistance, which is especially convenient as it allows to convert a multi-layer enclosing structure into a single-layer [19,20].

If the limits of variation of Pe and Po are known, then the sign of the signature in the boundary-value problem can be omitted and these criteria can be considered only in the closed interval $[0,1]$, then the Peclet and Pomerantsev criteria can be written as: $\overline{Pe} = (Pe - \inf Pe) / (\sup Pe - \inf Pe)$, $\overline{Po} = (Po - \inf Po) / (\sup Po - \inf Po) \in [0,1]$. In this case, all dependent and independent variables and parameters of the posed boundary-value problem are dimensionless and lie in a four-dimensional normalized unit space $(T, \overline{R}, \overline{Pe}, \overline{Po})$. The given transformations considerably simplify mathematical formalization of problems, eliminate physical dimensions and signs, and solve the issues of large-scale transition. The only thing that complicates the physical interpretation of problems, especially when graphic solutions to problems are built in the above space, where in fact the directionality of the flows and the sign of the heat source are "lost" due to the absence of negative values of the problem parameters in the closed interval $[0,1]$, but this complication is easily eliminated by returning to the initial parameters of the posed physical or applied boundary-value problems.

3. Conclusions

A generalized MM of heat and mass transfer in piecewise homogeneous media for hyperbolic (reflective high-temperature, high-speed and high-intensity processes), parabolic and elliptic types under various single-valuedness condition is presented.

Boundary-value problems of both interconnected and unconnected stationary and non-stationary transfer and some algorithms of their solution for classical form bodies are considered.

Analytical solutions of direct boundary-value problems of the processes of transfer of substances are obtained under generalized conditions on the outer contour of the investigated region and its discontinuous physical properties inside, as well as with variable (in time) transfer potentials in the boundary conditions (first, second, third and mixed kinds).

Formalized MM, analytical and approximate solutions of the boundary-value transfer problem are normalized to the criterial form, which is convenient for large-scale transitions, practical applications, parametric analysis of the obtained solutions, setting objectives for optimization and automation of control systems. Based on the results of solving a number of applied boundary-value problems, their physical interpretation is given.

4. Designations

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].

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The theory of transfer processes with short-term contact phases

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Abstract: Using the methods of systemic, mathematical and numerical analysis, as well as general physicochemical and thermodynamic laws, a complex of theoretical and experimental studies of transfer processes during short-term contact of phases has been carried out. These studies made it possible to fully reveal the regularities of external and internal heat and mass transfer, to find scientifically grounded ways to intensify the processes of vacuum, conductive and combined drying methods. Within the framework of linear nonequilibrium thermodynamics, a mathematical model of filtration-diffusion energy and mass transfer has been developed with a correct estimate of the orders of the terms in the system of differential equations of energy and mass transfer, taking into account the composition of the vapor-air mixture in the capillary-porous body. The limits of applicability of the hypothesis of short-term contact of phases according to the Fourier criterion for the transfer inside and outside the surfaces of the canonical shape (plate, cylinder, sphere) and wedge are estimated from the standpoint of the accuracy of calculating interphase flows. It is shown that in a number of cases the contact is not short-lived due to the curvature and the presence of angles on the contact surface, and not due to the finiteness of the dimensions of the contacting phases.

KEY WORDS: DRYING, DYNAMICS, SHORT-TERM CONTACT, PHASE, SURFACE, FOURIER CRITERION, MATHEMATICAL MODELING, HEAT AND MASS TRANSFER, ANALYSIS.

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 mainly determined by interrelated processes occurring inside the contact (boundary) layer of the material being processed (heat and mass transfer) and in the boundary layer of the environment (heating wall, air, inert coolant, steam, catalyst, etc.), since changes in environmental parameters change the conditions for the transfer of matter in the whole system, and the intensification or decrease in the material of physicochemical and phase transformations affects the structure of the boundary layer. A 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 investigate the kinetics and dynamics of the process and outline the optimal conditions for its implementation. Modern intensification of materials processing technology leads to an increase in the role of non-stationary interconnected exchange processes in comparison with stationary unrelated ones. This fact has not yet found sufficient reflection in the field of solving problems of energy and mass transfer at low Fourier numbers - with short-term contact of the phases.

2. Theory and results

One of the effective means of intensifying the transfer processes, for example, with a conductive energy conduit, is mixing the product, which constantly renews the contact layer of the material and equalizes the temperature, pressure, concentration of the processed medium (possibly three-phase) in its bulk, which makes it possible to obtain large flows through the interface. Often the physical model of these processes is a series of short-term contacts product with heating surface, and the transfer rate strongly depends on the contact time τ_k . For example, for drum, rake, roller, cylindrical dryers, where mixing is associated with rotation, τ_k is defined by the formula $\tau_k = \psi/\omega$ where ω is the angular velocity of rotation of the mixing devices, and ψ is the characteristic angle. For shelf dryers, belt dryers, disc dryers, vibrating dryers, etc. depending on the organization of mixing τ_k determined by the period of shaking, the frequency of vibration, the residence time of the product on a given plate, conveyor belt, etc. In the packet theory of fluidized and in the simplified model of gushing beds τ_k is determined by the speed of movement of the product (package) on the heating surface [8,9].

Let us consider separately the physical and mathematical aspects of modeling transfer processes during short-term contact of phases. Physical model of short-term contact of phases. Multiple repetition of contact interactions up to several thousand times makes it possible to describe heat transfer as stationary, using the heat transfer coefficient, the values of which are determined by unsteady heat and mass transfer during one contact.

Methods of organizing the contact of the product with the heating surface. In the analysis of short-term contact, the concept of heat transfer coefficient is introduced [3].

$$\alpha(\tau) = \frac{q(\tau)}{F(T_{\text{rn}} - T)}, \#$$

and it is called instant [8], conditional [10], contact [9], given [5]. For the average value $\alpha(\tau)$ for the time of one contact, the expression [3,7,8,10] is used

$$\langle \alpha^k \rangle_{\tau_k} = \frac{1}{\tau_k} \int_0^{\tau_k} \alpha(\tau) d\tau = 2 \frac{\sqrt{\lambda c p_0}}{\sqrt{\pi \tau_k}}, \#(2)$$

where λ is the coefficient of thermal conductivity, $\sqrt{\lambda c p_0}$ is the coefficient of heat assimilation (thermal activity) of the product [6]. Formula (2) was obtained by O. Krisher [3] under the following assumptions due to the small thickness of the heated contact layer of the material. A flat heating surface is placed at the point $x = 0$, and the material occupies the entire half-space $x > 0$; the heat conduction problem is one-dimensional, i.e. isothermal surfaces are parallel to the heating surface. The initial temperature distribution is assumed to be uniform, due to the presence of mixing:

$$T(x, 0) = T_0. \#(3)$$

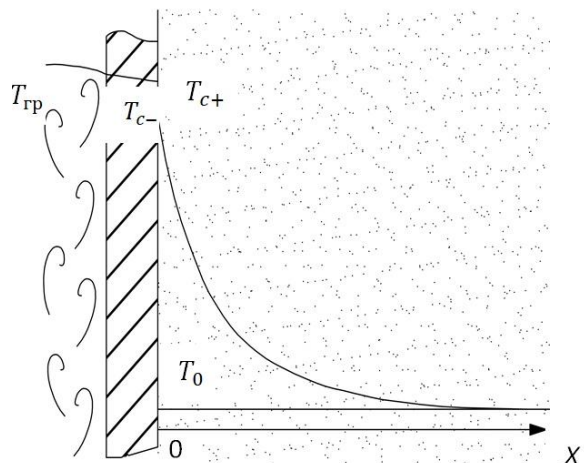


Fig. 1. On the formulation of the problem of short-term contact. Since the main thermal resistance is concentrated in the contact layer of the material, where the temperature gradients are many times higher than those in the heating agent and the shell, the temperature T_c is assumed to be constant, and T_c is considered in the first approximation to coincide with $T_c(T_{\text{rn}})$. The condition for the applicability of (2) in [3, 7, 10] is assumed (in the dimensions of the SI system) the inequality

$$Fo_k = \frac{a \tau_k}{H^2} \leq 0,106. \#(4)$$

which is fulfilled as equality when the temperature at the outer boundary of the body changes by $0,03 |T_{\text{rn}} - T_0|$. Here $a = \lambda/cp_0$

is the thermal diffusivity, H is the thickness of the material layer, which either changes in an obvious way, or requires some kind of averaging. The averaged values of H for cylindrical dryers are given in [7]. Through the criterion Fo_k , expression (2) can be represented in the form

$$\langle \alpha^k \rangle_{\tau_k} = \frac{2\lambda}{H\sqrt{\pi Fo_k}}.$$

In many devices, the heating surface is often curved, and the limitations of the applicability of the short-term contact model may be determined not by the thickness of the H layer, but by the curvature of the heating surface R . Estimates of type (4), taking into account the curvature of the heating surface, will be obtained below. In addition, it is known that internal evaporation, thermal diffusion, filtration of moisture contribute to heat transfer, and (2) was obtained by solving the problem of pure thermal conductivity. Finally, the coefficient $\langle \alpha \rangle$ is influenced by the composition of the remote multicomponent liquid mixture [11 - 15]. Taking these effects into account is an urgent task for the development of technological calculation and analysis of local changes in temperature and composition of the liquid phase of products. The physical model of short-term contact of phases is a powerful tool for analyzing transfer processes, since in a number of cases it has properties that make it possible to obtain relatively simple solutions of the posed boundary value problems, including multi-frontal problems of the Stefan type (freezing (thawing), evaporation, drying, filtration, sorption, adsorption, crystallization, etc.)

Mathematical models, self-similarity and invariants of solutions. In the general case, any mathematical description of processes in heterogeneous media, which include wet dispersed materials (suspensions), is based on the phenomenological theory of the multi-velocity continuum and is represented as a system of balance equations for conservation of mass, momentum, and energy. Further, depending on the considered medium and process, the multi-fluid (multi-velocity) model is generalized and closed (concretized) by attracting the mechanical and thermodynamic properties of the phases.

In the framework of nonequilibrium thermodynamics [16-17], on the basis of integral conservation laws, the interrelated heat and mass transfer in stationary dispersed media and capillary-porous bodies containing multicomponent liquid mixtures can be described using the following inhomogeneous system of nonlinear parabolic equations written in the vector-matrix form and resolved with respect to time derivatives (in this form, they are usually given by the system of differential equations of the transport theory).

$$C \frac{\partial \vec{\Pi}}{\partial \tau} = \text{div}(L \text{grad} \vec{\Pi}) + \vec{I}, \quad \#(5)$$

where $\vec{\Pi}$ is the n -dimensional vector of transfer potentials, L is the matrix of kinetic coefficients, C is the diagonal matrix of capacitance coefficients, I is the power vector of sources (or sinks). If there is an interaction of two phases, then in (5) the index $i = 1, 2$ is added, which we omit to simplify the notation, the operators of divergence and gradient are applied in (5) separately to each component of the corresponding vectors. It should be noted that system (5) can be written with respect to each of the interacting phases with the corresponding boundary conditions of uniqueness, including at the interface, similarly multi-frontal problems of the Stefan type. If the presence of sources is caused only by liquid-vapor phase transitions, and the vector of potentials includes the vector of moisture contents of the components U_x or the total moisture content U , then the vector I can be excluded from (5). To do this, it is sufficient to use the method of introducing the criterion of internal evaporation (phase transformation) ε , which is the ratio of the change in moisture content due to evaporation to its total change U_T , which is widespread in the theory of drying. In the case of an multicomponent liquid mixture, the ε values for the components can be different, this criterion will be a vector. After introducing ε from (5), within the framework of the model of short-term contact of phases, we obtain

$$C \vec{\Pi}_T = (L_\varepsilon, \vec{\Pi}_x)_x, \quad \#(6)$$

where L_ε is a matrix of kinetic coefficients that takes into account phase transitions. In the case when C and L_ε do not explicitly depend on coordinates and time (an explicit dependence on the complex $x/\sqrt{\tau}$ is admissible), but are functions of transport potentials, the Boltzmann substitution $\xi = \frac{x}{2\sqrt{\tau}}$ reduces (6) to a nonlinear system of homogeneous second-order ordinary differential equation

$$2\xi C \vec{\Pi}' + (L \vec{\Pi}) = \vec{0}, \quad \#(7)$$

Here and in what follows, the prime means differentiation with respect to ξ , and the subscript ε for L is dropped.

Using the assumption of the uniform distribution of $\vec{\Pi}$ at the time $\tau = 0$, we obtain the boundedness condition as $\xi \rightarrow \infty$

$$\vec{\Pi}(\infty) = \vec{\Pi}_0, \quad \#(8)$$

When formulating the boundary conditions in the form

$$P^{II} - \vec{\Pi}(0) = \vec{\Pi}_C, \quad \#(9)$$

(the task of linear relationships of the $\vec{\Pi}$ components on the heating surface) or

$$P^{II} \cdot L \vec{\Pi}'(0) = \vec{0}, \quad \#(10)$$

(the condition of impermeability of the heating surface for certain flows) the entire problem of short-term contact of phases (7) - (10) becomes self-similar. In (9) P^I and in (1.10) P^{II} are orthogonal projectors, not necessarily orthogonal to each other ($P^I \cdot P^{II} \neq 0$). In the case when the fluxes of energy or matter through the HP are specified, the condition for self-similarity is their proportionality $\tau^{-0.5}$ [21].

When solving problems with equations of the type (6) in the region $x > 0$, $\tau > 0$, most researchers use in addition to the initial and boundary conditions of semi-boundedness (or conditions at infinity) as $x \rightarrow \infty$ in three different forms:

$$\vec{\Pi}_x(\infty, \tau) = \vec{0}, \vec{\Pi}(\infty, \tau) = \vec{\Pi}_0, \lim_{x \rightarrow \infty} \vec{\Pi}(x, \tau) = \vec{\Pi}_0, \quad \#(11)$$

The last two conditions in (11) for the self-similar problem coincide with condition (1.8), which reflects the initial state of the product. Therefore, additional conditions of semi-boundedness were not considered.

In the case of constants L and C , which is most studied in the theory of drying when removing individual liquids, the problem of short-term contact of phases becomes linear and greatly simplified. To solve such problems, the superposition method is often used [2, 6, 19]. Eigenfunction expansions and integral transformation methods provide systematic schemes for constructing such solutions.

If the matrix $C^{-1} \cdot L$ has real, positive and different eigenvalues v_i^2 , $i = \overline{1, n}$, the solution (7) - (10) by the superposition method is reduced to finding the constants A_i in the representation

$$\vec{\Pi}(\xi) = \vec{\Pi}_0 + \sum_{i=1}^n A_i f_i \text{erfc}\left(\frac{\xi}{v_i}\right), \quad \#(12)$$

from the conditions on the heating surface (9) and (10). In (12), the linearly independent eigenvectors f_i of the matrix $C^{-1} \cdot L$ correspond to the eigenvalues v_i^2 . Direct verification can make sure that when specifying $\vec{\Pi}(\xi)$ in the form (12), equation (7) and condition (8) are satisfied automatically.

The constancy of L and C is an idealization of real relationships, however, it provides rich material for a qualitative analysis of the influence of various parameters on the transfer process. At the same time, even without this condition, the model of short-term contact due to the self-similarity of the problem

(7) - (10) has great advantages. Self-similar solutions can be used as "standards" in evaluating approximate methods for solving more complex problems; in addition, self-similarity simplifies the calculation and presentation of the characteristics of the phenomenon. In particular, assuming only the existence of a solution $\vec{\Pi}(\xi)$ one can establish the existence of a series of invariants of internal heat and mass transfer.

An integral component of $\vec{\Pi}$ in a non-isothermal process is temperature T , and its change at any point in the material can be considered monotonic: $T_\tau(x, \tau) > 0$ during heating. Therefore, from the solution $T(\xi)$, one can obtain a unique dependence $\xi(T)$ and write $\vec{\Pi} \rightarrow \vec{\Pi}(T)$ in the form

$$\vec{\Pi}(\xi) = \vec{\Pi}(T), \quad \#(13)$$

Thus, in the theory of short-term contact of phases, there are $n - 1$ invariants of internal interconnected heat and mass transfer, according to the number of acting potentials that determine this transfer. The relationships between the local values of temperature, moisture content, composition of the multicomponent liquid mixture and pressure, which are independent of time and coordinates, can serve to analyze the combined effect of heating and dehydration in various technological processes. Such an analysis is especially relevant for biological products, since their thermal and xerolability is due precisely to the combined effect of these factors.

In connection with the large role of the model of short-term contact of phases in the study of processes with stirring, a more detailed analysis of the limits of applicability of this model is required.

The limits of applicability of the model of short-term contact of phases. The conditions under which the contact can be considered short-term depend on what characteristics of the contact are being investigated. O. Krisher's restriction (4) is associated with a change in temperature on the free surface of the body by 3% of the total temperature head, and is used as a characteristic of the applicability of formula (2) for the heat transfer coefficient. It is of interest to elucidate the influence of the finiteness of body dimensions and the shape of the heating surface directly on the heat transfer coefficient. Let us consider in the framework of pure thermal conductivity the

problems for an unbounded plate ($G = 0$), an infinite cylinder ($G = 1$) and a ball ($G = 2$) - Fig.2.

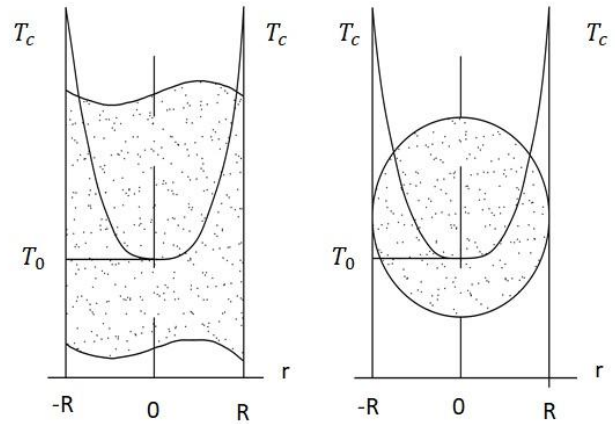


Fig. 2 On the formulation of heat conduction problems for bodies of canonical form

All three tasks have a common formulation

$$T_r - a \left(T_{rr} + \frac{r}{r} T_r \right) = 0, \#(14)$$

$$T(r, 0) = T_0, \quad T(\pm R, T) = T_c$$

and the same kind of solution [6]:

$$T(Fo, \eta) = T_c + (T_0 - T_c) \sum_{i=1}^{\infty} A_i \varphi(\mu_i \eta) \exp(-\mu_i^2 F_j), \#(15)$$

Where

$$\eta = \frac{r}{R},$$

$$F_j = \frac{a\tau}{R^2}, \#(16)$$

and μ_i - are the positive roots of the characteristic equation numbered in ascending order

$$\varphi(\mu) = 0.$$

The eigenfunctions of problems (14) and the coefficient A_i are determined by the formulas in Table. 1.

Table 1. Parameters of solutions for heat conduction

G	0	1	2
$\varphi(\mu_i \eta)$	$\cos(\mu_i \eta)$	$J_0(\mu_i \eta)$	$\frac{\sin(\mu_i \eta)}{\mu_i \eta}$
A_i	$(-1)^{i+1} \frac{2}{\mu_i}$	$\frac{2}{\mu_i J_1(\mu_i)}$	$(-1)^{i+1} \cdot 2$

Here J_0 and J_1 are the Bessel functions of the first kind of the zero and first orders, respectively. Taking into account the Fourier law, α (τ) is determined by the value

$$\alpha(\tau) = \frac{\lambda}{R(T_c - T_0)} T_{\eta=1} |_{\eta=1}. \#(18)$$

Formal term-by-term differentiation of series (15) at different G gives a general expression

$$\alpha(\tau) = \frac{2\lambda}{R} \sum_{i=1}^{\infty} \exp(-\mu_i^2 F_o), \#(19)$$

in which the shape of the heated body is reflected only through the sets μ_i $i=1,2, \dots$ Formal term-by-term integration (19) in accordance with (2) gives

$$\langle \alpha \rangle_{\tau_k} = \frac{2\lambda}{R F_{ok}} \sum_{i=1}^{\infty} \frac{1 - \exp(-\mu_i^2 F_{ok})}{\mu_i^2}. \#(20)$$

A discussion of the convergence of series (19), (20) and estimates of their remainders are given in [1]. Note that the summation of these series in the problem of short-term contact of phases must be carried out at small F_o , when there is no predominance of the first terms. Therefore, the numerical calculation of the sums (19), (20) was carried out on the basis of a given maximum permissible relative inaccuracies $\delta = 10^{-3}$. Separate task is the calculation of

several hundred roots J_0 (it is precisely these quantities that are necessary for $\delta = 10^{-3}$). This problem was solved sequentially in i , starting with the value $\mu_1 \approx 2,4$. The iterative rule of false position was used, and for the localization of the roots, the segments

$$\mu_{i+1} \in \left[\mu_i + \pi - \frac{0,1415}{i}, \mu_i + 3,1416 \right],$$

the position of which is associated with the almost periodic nature of the growth of μ_i [19]. Due to the precise localization of the roots, their values were calculated with a relative error of no more than 10^{-6} for 2 - 3 iterations, with this level of error it was possible to determine 250 roots. The results coincide with the above accuracy with the data [19], where the first 60 roots of J_0 with 5 - 7 significant digits are given.

However, it should be noted that the classical solution in the Fourier form, consisting of the product of two functions, taking into account, respectively, the change in temperature in time and along the radius (thickness), is convenient for large F_o . For small F_o , solutions obtained by methods of operational calculus are convenient, in particular, solutions in the Laplace form (Laplace transform), which represent the well-known combination of the functions erf and erfc. In these cases, you can always limit yourself to a few first (or only the first) members of the series, discarding all the rest. In addition, operational methods make it possible to obtain a number of approximate solutions with any degree of accuracy, which are quite simple and can be used in technical calculations. An analysis of the obtained expressions $\alpha(F_o)$ for various G shows that

$$\lim_{F_o \rightarrow 0} \left[\frac{\alpha(F_o)}{\alpha^k(F_o)} \right] = 1,$$

those. the formulas for calculating α (τ) for small F_o asymptotically coincide with the formulas used to calculate α^k (τ).

By generalizing (4) to. the case of multicomponent energy and mass transfer in a plate is the same condition, in which, instead of the thermal diffusivity (or diffusion) coefficient, one should use the largest of the eigenvalues of the matrix $C^{-1} L$ [22]. Depending on the objectives of the study, the level of permissible fluctuations of various components Π at the outer boundary $x = \Pi$ can be different, therefore, it is possible to weaken or strengthen condition (4), or a combination of this type of conditions. In a specific case, such estimates are carried out quite simply using solutions of the form (12).

The same approach is obviously extended to the case of contact between two plates of finite thickness. However, the very origin of the condition - guaranteeing the accuracy of the calculation of the potential fields in a plate of finite dimensions - has disadvantages. It is not connected with the main task of calculating energy and mass transfer with the determination of the intensity of metabolic processes and therefore does not say anything about the accuracy of calculating the fluxes of transported substances.

In addition, in real situations, a limitation associated with the curvature of the contact surface (the surface of a granule, a gas bubble, a cylindrical shell, etc.), and not with the surface of the dimensions of the contacting bodies, may be active. A significant limitation can also be the presence of two generators of length l during the contact time of the heat flux through the surface; consideration of the asymptotics as $k \rightarrow \infty$ and the subsequent approximation make it possible to determine the desired error.

When evaluating heat transfer from a cylinder of circular cross section and a sphere to the outer region, the solution was used [23]. In fig. 3 the calculated dependences of the ratio of the heat transfer coefficient to its base value calculated for the flat boundary of the half-space according to O. Krisher [3] are constructed.

As can be seen from the figure, the model of short-term contact of phases is suitable for estimating $\alpha > \alpha_{\tau_k}$ at larger Fo than in the case of estimating $\alpha(\tau)$ - regardless of the shape of the heating surface. With an approximate coincidence of the characteristic size of the body H with the radius of curvature of the heating surface R , the applicability of the model of short-term contact of phases is limited precisely by the presence of the curvature of the heating surface. For roller dryers $H \ll R$ it is necessary to analyze the influence of both factors. For dryers with flat heating surfaces - the applicability of the model of short-term contact of phases is determined by the thickness of the product layer. Fig. 3 it can also be seen that Krisher's constraint (4) is unreasonably strict for engineering estimates of heat transfer from a flat heating surface.

For example, for industrial drum and rake dryers, the τ_k value does not exceed 60 s. For $a = 10^{-7} \text{ m}^2/\text{c}$ and the radius of curvature of curvature of the heating surface $R = 1 \text{ m}$, the corresponding Fo_k do not exceed $6 \cdot 10^{-6}$, then is the influence of the curvature of the heating surface in accordance with table. 2 can be neglected. Taking the average thickness of the product layer $H = 0.2 \text{ m}$, we get $Fo_0 \leq 1,5 \cdot 10^{-4}$. Thus, for these dryers, the application of the short-term contact model can be considered justified.

The maximum thickness of the layer heated by 3% of the total temperature head, in accordance with (4), here is no more than 8 mm. However, for cabinet, roller, etc. devices with a small layer thickness H , the question of the applicability of the short-term contact model requires a separate analysis in each case. In the presence of a large number of mates of the heating surface with small radii of curvature, additional analysis based on table. 2 may be needed for drum and stroke.

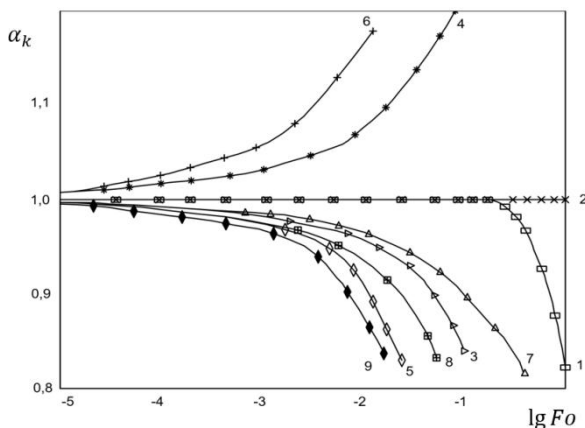


Fig. 3. The ratio of the calculated heat transfer coefficient to its value according to O. Krisher, depending on the Fourier number during heat transfer: 1.2 - respectively, into the interior and exterior of an infinite plate; 3.4 - into the interior and exterior of an endless cylinder; 5.6 - into the interior and exterior of the sphere; 7,8,9 -

into the inside of an unlimited wedge with an opening angle of 150, 120 and 90 °, respectively.

Coefficient heat transfer	Heating surface shape	Plane		Cylinder		Sphere	
	Error level, %	3	5	3	5	3	5
$\alpha(\tau)$	$F_{0_{max}} \cdot 10^{-3}$	247	279	1,12	3,09	0,269	0,646
$\alpha(\tau_k)$	$F_{0k_{max}} \cdot 10^{-3}$	447	537	4,47	1,2	1,26	3,35

Table 2. The largest Fourier numbers at which the relative error in calculating α according to Krisher's formulas does not exceed 3% and 5%

When switching to multicomponent transfer, for a rough estimate, you can also substitute v_{max}^2 for a (or D). When considering the heat and mass transfer in two contacting phases, a more specific analysis is required, however, here v_{max}^2 plays a decisive role as well. devices.

3. Conclusions

The limits of applicability of the hypothesis of short-term contact of phases according to the Fourier criterion for the transfer inside and outside the surfaces of the canonical shape (plate, cylinder, sphere) and wedge are estimated from the standpoint of the accuracy of calculating interphase flows. It is shown that in a number of cases the contact is not short-lived due to the curvature and the presence of angles on the contact surface, and not due to the finiteness of the dimensions of the contacting phases.

Within the framework of linear nonequilibrium thermodynamics, a mathematical model of filtration-diffusion energy and mass transfer has been developed with a correct estimate of the orders of the terms in the system of differential equations of energy and mass transfer taking into account the composition of the vapor-air mixture in a capillary-porous body.

Depending on the value of the phase transformation criterion, the system of differential equations is simplified to three different systems of equations with the number of coupled equations in each no more than 2, describing the fields of temperature, humidity (concentration) and pressure, and the eigenvalues of the matrices of their coefficients are real, positive and different.

It has been established that during the transfer of a liquid, in the main one, in the form of vapor, the filtration-diffusion heat and mass transfer is expressed by the equations of diffusion heat and mass transfer with an increased coefficient of mass conductivity.

Boundary-value problems of diffusion and diffusion-filtration heat and mass transfer are solved under mixed boundary conditions of the first and second kind, on the basis of which integral kinetic dependences of drying processes (drying and heating rates), formulas for calculating heat and mass transfer coefficients, Rebinder numbers, temperature coefficients and subkinetic drying parameters.

Thus, a complex of theoretical and experimental studies has been carried out.

(using the methods of systemic, mathematical and numerical analysis, as well as general physicochemical and thermodynamic laws) transfer processes during short-term contact of phases (using the example of vacuum, conductive and combined drying methods), which made it possible to most fully reveal the laws of external and internal heat and mass transfer, to find scientifically grounded ways to intensify the considered processes

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Field-free calculation of heat and mass transfer flows with short-term contact of phases

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Abstract: Calculation of thermal diffusion and filtration fluxes at the interface by "traditional" methods requires preliminary determination of the potential values (concentration, moisture content, temperature, pressure) in the four-dimensional space of events. Such methods for solving boundary value problems, which provide "extra" information for technical calculations, are usually very laborious and require the use of numerical methods that are not always convenient in engineering practice. The proposed fieldless calculation method allows one to determine on the boundary of the region the gradients from the transfer potentials and, consequently, energy and material flows in the form of a known functional of the potentials at the interface at their short-term contact directly on the matrix of transfer coefficients of the formalized boundary value problem. This method uses the fractional index differentiation operation (fractional differentiation) and is convenient for solving limiting boundary value problems, i.e. when the characteristic size of the contacting phases in the boundary conditions of boundary value problems tends to infinity or the time of their interaction tends to zero.

KEYWORDS: DRYING, DYNAMICS, SHORT-TERM CONTACT, PHASE, SURFACE, FOURIER CRITERION, MATHEMATICAL MODELING, HEAT AND MASS TRANSFER, ANALYSIS

1. Introduction

Calculation of thermal diffusion and filtration flows at the interface by "traditional" methods requires a preliminary determination of the value of the potentials P^- (concentration, moisture content, temperature, pressure) in the four-dimensional space of events $R^4(x_1, x_2, x_3, \tau) = R^4(\bar{x}, \tau)$ [1,2]. Such methods for solving boundary value problems, which provide "extra" information for technical calculations, are very laborious and require the use of numerical methods that are not always convenient in engineering practice [2,3]. The field-free calculation method allows one to determine the gradients from the transfer potentials at the boundary of the region $(\bar{x}|_{\bar{x}=0})$ at their short-term contact directly on the matrix of transfer coefficients of the formalized boundary value problem. This method uses the fractional index differentiation operation [4].

2. Materials and methods

We present briefly the necessary information about their theory of fractional differentiation.

Definition. For function $f(x)$, given on the segment $[a, b]$, each of the expressions

$$(D_{a+}^{\alpha} f)(x) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_a^x \frac{f(t) dt}{(x-t)^{\alpha}}, \quad (1)$$

$$(D_{b-}^{\alpha} f)(x) = -\frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_x^b \frac{f(t) dt}{(t-x)^{\alpha}}, \quad (2)$$

is called the fractional derivative or the Riemann-Liouville derivative of order α , $0 < \alpha < 1$, respectively left-sided right-sided. Γ (1) and (2) Γ - gamma function, $f(x)$ - piecewise continuous function.

Let us give a sufficient criterion for the existence of fractional derivatives.

Lemma. If a $f(x)$ belongs to the class of absolutely continuous on the segment $[a, b]$ functions, then $f(x)$ almost everywhere has derivatives $D_{a+}^{\alpha} f$ и $D_{b-}^{\alpha} f$, $0 < \alpha < 1$, moreover $D_{a+}^{\alpha} f$ и $D_{b-}^{\alpha} f$ belong to the class measurable on $[a, b]$ function $f(x)$ ($L_r(a, b)$, $1 \leq r < 1/\alpha$), for whom $\int_a^b |f(x)|^r dx < \infty$ and

$$D_{a+}^{\alpha} f = \frac{1}{\Gamma(1-\alpha)} \left[\frac{f(a)}{(x-a)^{\alpha}} + \int_a^x \frac{f'(t) dt}{(x-t)^{\alpha}} \right], \quad (3)$$

$$D_{b-}^{\alpha} f = \frac{1}{\Gamma(1-\alpha)} \left[\frac{f(b)}{(b-x)^{\alpha}} + \int_x^b \frac{f'(t) dt}{(t-x)^{\alpha}} \right]. \quad (4)$$

The fractional Liouville derivatives for the semiaxes with the corresponding limits of integration in (1) and (2) are introduced similarly.

3. Theory

Let us consider a mathematical model of interconnected unsteady heat and mass transfer under conditions of short-term contact interaction of phases, which, within the framework of the formalism of linear nonequilibrium thermodynamics based on integral conservation laws, is formulated as a system of linear homogeneous

differential equations in the following compact vector-matrix form [5]:

$$\begin{cases} \bar{\Pi}_{j\tau} = K_j \Delta \bar{\Pi}_j, & x \in (0, (-1)^j \infty), \tau \in (\tau_0, \tau_k), j=1, 2 \\ \bar{\Pi}_j(x, \tau_0) = \bar{\Pi}_j(x, \tau_k) = \bar{\Pi}_j \left[(-1)^j \infty, \tau \right] = \bar{\Pi}_{j0}, & |x| \end{cases} \quad (5)$$

$$\begin{cases} k_1 \bar{\Pi}_{1x}(0, \tau) = k_2 \bar{\Pi}_{2x}(0, \tau), \end{cases} \quad (6)$$

where $\bar{\Pi}_j, \bar{\Pi}_{jx}$ - local changes in the vector of transfer potentials $\bar{\Pi}$ dimensions n_j respectively in time τ and coordinate x in j phase, $K = kC^{-1}$ - constant matrix of system parameters ($n \times n$), k, C^{-1} - matrices of kinetic coefficients and inverse diagonal matrix of capacitance coefficients, respectively, Δ - component-wise Laplacian, x - coordinate normal to the plane of contact with zero at the interface, τ_k - duration of contact.

In what follows, omitting the indices of the contacting phases and setting for definiteness $x \in (0, \infty)$, $\tau_0 = 0$ and $\bar{\Pi}(0, \tau) = \bar{\Pi}_s$, we introduce a new vector variable $\bar{\theta} = \bar{\Pi}_0 - \bar{\Pi}$ (bringing constant initial conditions to zero) and expand the difference between differential operators in time and coordinate in (5) similarly to the difference of squares, then system (5) - (7) will be rewritten as:

$$\begin{cases} (\partial_{\tau}^{0.5} - \sqrt{K} \partial_x)(\partial_{\tau}^{0.5} + \sqrt{K} \partial_x) \bar{\theta} = \bar{\theta}, \\ \bar{\theta}(x, 0) = \bar{\theta}(\infty, \tau) = \bar{\theta}, \\ \bar{\theta}(0, \tau) = \bar{\theta}_s(\tau). \end{cases} \quad (8)$$

$$\bar{\theta}(x, 0) = \bar{\theta}(\infty, \tau) = \bar{\theta}, \quad (9)$$

$$\bar{\theta}(0, \tau) = \bar{\theta}_s(\tau). \quad (10)$$

If the elements of the matrix $k_{ij} > 0$ and $\det K > 0$, then the definition of the radical from the matrix is carried out in a continuous unambiguous manner [4]. When the matrix has dimensions 2×2 , then the corresponding formulas for determining the radical from the matrix are:

$$b_{11}^2 = [k_{11}(k_{11}-k_{22})^2 + k_{12}k_{21}(3k_{11}-k_{22}) + 2k_{12}k_{21} \sqrt{(k_{11}k_{22}-k_{12}k_{21})}] \Delta^{-1},$$

$$\sqrt{K} = \begin{pmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{pmatrix}^{\frac{1}{2}} = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}, \quad (11)$$

where $k_{ij} > 0, k_{11}k_{22} > k_{12}k_{21}$,

$$b_{22}^2 = b_{11}^2 - (k_{11} - k_{22})$$

$$b_{12} = \frac{k_{12}}{b_{11}+b_{22}}, b_{21} = \frac{k_{21}}{b_{11}+b_{22}}, b_{11} > 0, b_{22} > 0, \Delta = (k_{11}-k_{22})^2 + 4k_{12}k_{21}.$$

In this case, under conditions of linear nonequilibrium thermodynamics, the matrix K , due to the positiveness of the production of entropy, must be positively determined, that is, the following conditions must be satisfied [7-9]:

$$k_{11} > 0, k_{22} > 0, (k_{12}+k_{21})^2 < 4k_{11}k_{22}. \quad (12)$$

Thus, according to the second law of thermodynamics, "eigencoefficients" (or direct coefficients, for example, the coefficients of thermal conductivity, diffusion), k_{ii} must be positive, and the "cross factors" (or drag factors, which are determined by superimposing effects such as thermal diffusion) k_{ij} ($i \neq j$) can have any sign. Moreover, due to microscopic

reversibility [7], the elements k_{ij} must satisfy the Onsager relation, $k_{ij} = k_{ji}$, that is, the matrix is symmetric, and in this case, inequality (12) implies the first inequality in (11) and as a consequence, $b_{12} = b_{21}$. Physically diagonal coefficients k_{ii} determine the intensity of transfer of the i -th flow of a substance (heat, mass of a substance) under the direct action of the thermodynamic force of the same name (for a heat flow, the thermodynamic force will be ∇T – temperature gradient, and for mass flow ∇C – concentration gradient).

Further, considering from physical considerations the equations formed by the right factor of the operator in (8) (the left factor with increasing, for example, the temperature at the interface gives $T_x|_{x=0} > 0$, which is physically absurd) and, writing the latter at $x = 0$, we obtain the relation defining $\vec{\theta}_s$ at the boundary of short-term contact of phases:

$$D^{0.5}\vec{\theta}_s(\tau) + \sqrt{K}\vec{\theta}_{sx}(0) = \vec{0}, \quad (13)$$

For fractional differentiation, the right-hand fractional derivative is used in (13).

The solution of the system of equations (13) with respect to energy and material flows no longer causes difficulties, since the formulas of the fieldless method are applicable to systems of differential equations of parabolic, and for high-intensity processes of heat and mass transfer and hyperbolic types. Calculations of fluxes and a number of heat-mass transfer characteristics for the system of equations (5) with boundary conditions of the first kind and the considered problems of molecular and molecular-molar transfer with mixed boundary conditions of the first and second kind, carried out by the field-free method, are fully confirmed by calculations performed on the fields of transfer potentials proposed in [5].

3. Conclusions

For limiting boundary value problems, the possibility of using a non-field method for calculating heat and diffusion fluxes at interfaces is shown, which essentially uses the operation of a differential fractional index, does not require preliminary determination of fields, allows one to obtain a solution in the form of finite formulas, and is important in applied research.

Analytical solutions of boundary value problems of diffusion and diffusion-filtration heat and mass transfer under mixed boundary conditions of the first and second kind and the calculation of heat and material flows from the obtained temperature and concentration fields are fully confirmed by calculations obtained by the fieldless method.

The results obtained serve the development of the general theory of mathematical modelling, are useful in the formulation of experimental studies on stationary and non-stationary energy and mass transfer, in the analysis and calculation of heat and mass transfer processes in applied research and design.

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Study on the effectiveness of integrated methodologies for determining thermophysical properties of building envelope structures

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Abstract: To design energy-efficient buildings, it is essential to accurately calculate, monitor, and analyze their energy consumption at all stages: from conceptual (sketch) development and design to construction and operation. However, current regulatory documentation lacks methodologies that fully account for the interrelated processes occurring in building envelopes—such as heat transfer, moisture accumulation, and air infiltration—evaluate the effectiveness of specific energy-saving measures, or perform energy consumption data analysis to determine a building's actual energy performance indicators. This highlights the relevance of calculating and analyzing building energy consumption while accounting for heat and mass transfer processes in envelope structures and the presence of various architectural and construction elements. A methodology has been developed for processing data obtained from building thermal energy metering systems. This methodology allows, during the operational phase, to determine buildings' energy characteristics, evaluate the efficiency of thermal energy use, and assess the effectiveness of energy-saving measures.

KEY WORDS: SHORT-TERM CONTACT, MATHEMATICAL MODELING, SYSTEMS OF DIFFERENTIAL EQUATIONS, POTENTIALS, PHASES, MODES, VECTOR, MATRIX, HEAT AND MASS TRANSFER, COEFFICIENTS.

1. Introduction

One type of energy-efficient building is the Passive House (Passivhaus). Passive Houses are buildings with extremely low energy demand, where annual heating energy consumption does not exceed 15 kWh/(m²·year), and heat losses through the building envelope are limited to a U-value ≤ 0.15 W/(m²·K).

Achieving these targets is impossible without using high-performance thermal insulation with a thermal conductivity $\lambda < 0.030$ W/(m·K), as well as design solutions that minimize thermal bridges and ensure airtightness.

Over the past five years, rapid advancements have been observed both in innovative insulation materials and intelligent insulation systems that combine energy efficiency, environmental sustainability, and durability.

2. Review of New Thermal Insulation Materials

Vacuum Insulation Panels (VIPs) remain at the forefront of thermal protection materials due to their exceptionally low thermal conductivity—ranging from 0.004 to 0.008 W/(m·K)—which is 5–10 times lower than that of conventional insulators [1].

Although VIPs were initially limited by high costs and significant degradation risks if the vacuum envelope was damaged, substantial progress in the 2020s has significantly improved their reliability, greatly expanding their application scope [2].

Researchers at Fraunhofer IBP have developed innovative VIPs with multilayer barrier envelopes based on recyclable polymers and nanofibrillated cellulose cores, extending the projected service life to over 30 years, even under high humidity and mechanical stress [1]. These panels are especially effective in thermal bridge-prone areas—such as window reveals and balcony junctions—and in historic building retrofits where wall thickness is critically constrained.

Silica aerogels, with thermal conductivity $\lambda \approx 0.012$ – 0.018 W/(m·K) and famously known as “solid smoke” due to their ultra-low density, have evolved from fragile monolithic forms to flexible composite blankets compatible with timber frames, curved surfaces, and render systems [3, 4].

Within the European AEROCOAT project, aerogel-based renders were developed for thermally upgrading historic façades, enabling compliance with Passivhaus standards without altering the building's external appearance, which is essential for structures in protected heritage zones [3].

Environmental sustainability—a core principle of the Passive House concept—has spurred the development of new bio-based materials that significantly outperform traditional cellulose and wood-fiber insulations.

Mycelium composites, made from fungal mycelium and agricultural waste, exhibit thermal conductivity $\lambda \approx 0.038$ – 0.045

W/(m·K), are fully biodegradable, and—when properly modified—show good fire resistance [5].

Alginate foams derived from seaweed, developed in 2023, achieved $\lambda \approx 0.032$ W/(m·K) combined with high moisture resistance—a rare combination for bio-based materials [6].

Compressed straw without synthetic binders is successfully used in monolithic walls, achieving U-values as low as 0.12 W/(m²·K). These materials not only reduce the carbon footprint but also help regulate indoor humidity and improve indoor climate [7].

Metal-Organic Frameworks (MOFs), particularly ZIF-8 (Zeolitic Imidazolate Framework), show strong potential for ultra-low-conductivity insulation. In 2024, researchers at ETH Zürich produced an MOF-based aerogel with $\lambda = 0.011$ W/(m·K) and high stability at relative humidity up to 80% [8]. While this technology has not yet reached industrial scale, it paves the way for next-generation “smart” insulation with adaptive properties.

Modern energy-passive houses increasingly employ dynamic insulation systems, notably Dynamic Insulation, in which outdoor air slowly passes through a porous insulation layer, reducing heat losses while providing natural ventilation [9].

Phase Change Materials (PCMs) are integrated into walls and ceilings to smooth daily temperature fluctuations—becoming especially relevant under climate change and increasing cooling demands [10].

3. Current Trends in Determining Envelope Structure Characteristics

According to ISO 9869-1:2014, still widely used today, key experimental methods for determining thermophysical properties include: Heat Flow Meter (HFM) method, Infrared Thermography (IRT), Calibrated Hot Box, Dynamic methods (reducing measurement time from weeks to hours) [11].

Recent years show a clear trend toward hybrid approaches combining multiple methods to improve measurement accuracy—especially under real-world building operating conditions.

Researchers at the Fraunhofer Institute for Building Physics conducted a large-scale field study in 12 certified Passive Houses in Germany, using the HFM method over 14–21 days with a temperature difference of at least 10 K. Results were compared with calculations per DIN EN ISO 6946 and BIM models accounting for thermal bridges [11].

The average deviation between measured and calculated U-values was +8%, indicating systematic underestimation of heat losses in design calculations. The largest discrepancies—up to 25%—occurred at window and balcony slab junctions due to insufficient modeling of linear thermal bridges. However, 3D thermal modeling (using ANSYS or Therm) reduced errors to <5%.

A team from Politecnico di Torino developed an automated thermogram analysis method using convolutional neural networks to estimate U-values and detect anomalies. Tested on 30 buildings (including EnerPHit retrofits), the method achieved ± 0.03 W/(m²·K) accuracy versus HFM and successfully identified hidden insulation defects—such as settling and moisture accumulation—that are invisible to visual inspection. Conventional models ignoring defects overestimated insulation performance by 12–18% [12].

Researchers at Empa proposed an accelerated “step heating” method: briefly heating the interior wall surface and analyzing the cooling curve. This reduces measurement time to 6–8 hours instead of the traditional 2–3 weeks. The method was tested on walls with aerogel and wood-fiber insulation, showing <7% deviation from ISO 6946 and HFM for homogeneous constructions. However, for multilayer systems with PCMs, deviations reached 15% due to unaccounted thermal inertia in steady-state calculations [13].

The IEA EBC Annex 80 project (completed in 2024) analyzed 3–5 years of monitoring data from 18 buildings and found that moisture accumulation in bio-based insulation increases thermal conductivity by 10–22%—a factor ignored in standard dry-state material calculations [14]. The authors recommend making dynamic hygrothermal modeling (e.g., using WUFI Pro) a mandatory part of Passive House design in temperate and humid climates.

In summary, modern thermophysical studies confirm that calculated U-values per ISO 6946 are often overly optimistic, especially when thermal bridges, installation defects, or material moisture are present. Thus, on-site measurements are essential to validate design solutions in Passive Houses. 3D thermal bridge modeling per ISO 10211 should become standard practice, not an exception. Dynamic methods and AI-driven technologies significantly accelerate and reduce the cost of diagnostics, enabling mass-scale application. Long-term monitoring—including in-wall humidity and temperature—is necessary to assess a building’s true energy performance.

4. Experimental Determination of Thermal Characteristics in a Climatic Chamber

A comprehensive experimental study was conducted on the thermal characteristics of prototype envelope structures and moisture distribution through their thickness.

A climatic chamber (Fig. 1) was used, retrofitted with an internal partition and equipment to maintain set microclimatic parameters in cold and warm compartments.

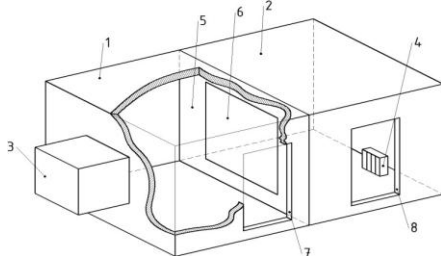


Fig. 1. Layout of the climatic chamber: 1 – cold compartment; 2 – warm compartment; 3 – refrigeration unit; 4 – heating device; 5 – dividing wall; 6 – test structure or material; 7, 8 – sealed doors to the cold and warm compartments.

Two types of prototype envelope structures were tested. The goal was to determine the thermo-hygric state of multilayer constructions under varying outdoor temperatures (simulating “cold waves”). Results are shown in Fig. 2, depicting temperature and humidity profiles through the wall thickness at different cold-chamber temperatures.

Thus, under laboratory conditions, “cold waves” of varying intensity and duration—typical of real winter conditions—were successfully replicated.

5. Specimens and Experimental Theirs Thermal Characteristics

Table 1 lists specimen characteristics and table 2 shows boundary conditions. Temperature and relative humidity profiles through the wall at different cold-chamber temperatures are shown in Figs. 2 and 3. Test durations: at $t_{ext} = -32^{\circ}\text{C}$: 58 h (2.4 days), $t_{ext} = -11^{\circ}\text{C}$: 100 h (4.2 days), $t_{ext} = -20^{\circ}\text{C}$: 176 h (7.3 days).

Table 1. Material Characteristics of the Envelope Structure

№	Material	Thickness m	Density kg/m ³	Thermal Conductivity W/(m·°C)	Water Vapor Permeability mg/m·h·Pa
1	Plaster	0.015	1800	0.93	0.09
2	Silicate brick masonry	0.25	1800	0.87	0.11
3	ROCKWOOL mineral wool	0.10	90	0.041	0.30

Table 2. Boundary Conditions at Inner and Outer Surfaces

Cold Chamber Temperature , °C	Inner surface		Outer surface	
	t_i , °C	ϕ_i , %	t_o , °C	ϕ_o , %
–32	18.1	78	–28.1	88
–11	15.5	54	–8.1	69
–20	14.3	63	–15.5	58

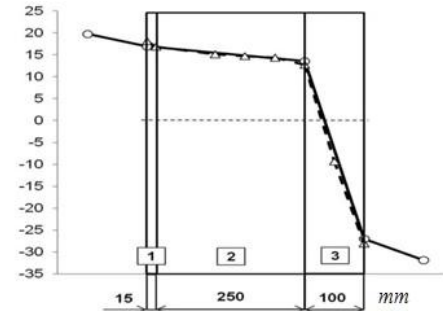
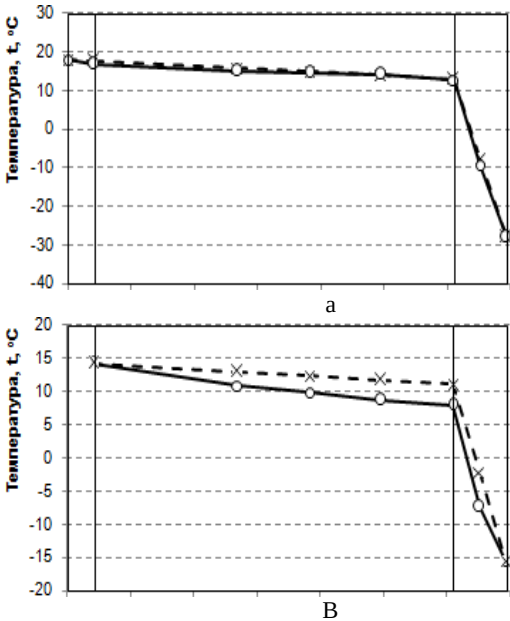


Fig. 2. Temperature distribution through the wall ($t_o = -32^{\circ}\text{C}$): 1 – plaster, 2 – brick masonry, 3 – mineral wool



Based on experiments, the following thermal characteristics were determined (Table 3a,b): thermal resistance of brick masonry (R_{bm}) and mineral wool (R_{mv}), thermal conductivity of brick (λ_{bm}) and mineral wool (λ_{mv}), inner surface heat absorption coefficient (α_i) and outer surface heat transfer coefficient (α_o):

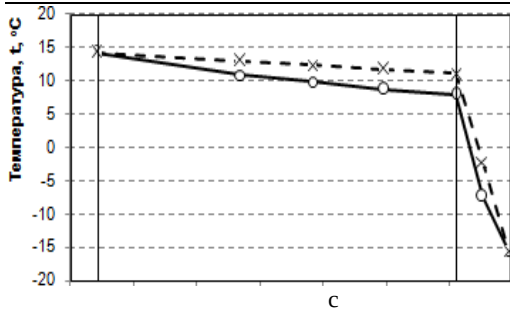


Fig. 3. Temperature profiles under different cold-chamber conditions (solid line – experiment, dashed – calculation):
(a) $t_0 = -32^\circ\text{C}$, (b) $t_0 = -20^\circ\text{C}$, (c) $t_0 = -11^\circ\text{C}$

Table 2. Experimental Thermal Characteristics

Temp, °C	q , W/m ²	R_{bm} , m ² ·°C/W	R_{mv} , m ² ·°C/W	
-32	32.5	0.128	1.254	
-11	47.8	0.111	0.384	
-20	63.3	0.101	0.370	
Temp, °C	λ_{bm} , W/(m·°C)	λ_{mv} , W/(m·°C)	α_b , W/(m ² ·°C)	α_o , W/(m ² ·°C)
-32	1.96	0.08	11.6	6.7
-11	2.25	0.26	5.8	15.9
-20	2.48	0.27	5.3	15.4

6. Mathematical Model of Unsteady Heat Transfer for a Brick Wall Envelope

Problem statement for a brick wall:

Initially, for a brick wall, we have:

$$\begin{cases} t_\tau = at_{xx}, x \in (0, h), \tau \in (0, T) & (1) \\ t(x, 0) = f(x) & (2) \\ -\lambda \nabla t(0, \tau) = \alpha_0 [\tilde{t}_0 - t(0, \tau)] & (3) \\ -\lambda \nabla t(h, \tau) = \alpha_h [t(h, \tau) - \tilde{t}_h] & (4) \end{cases}$$

In the building envelope, $\nabla_z t = \nabla_y t = 0$; $\nabla_x t \neq 0$ - thermal insulation condition (adiabaticity) of the wall, where $z = H$ - is the height of the building's ES, $y = L$ is the length of the building's ES, $x = h$ - is the thickness of the building's ES, $h \ll L$, $h \ll H$.

Constant but different temperatures are maintained on opposite surfaces of the ES:

$$t(0, \tau) = t_{w1};$$

$$t(h, \tau) = t_{w2};$$

and the initial wall temperature $t(x, 0) = t_{w0}$;

$$\infty \leftarrow \tau_1 > \tau_2 > \tau_3 > 0;$$

$$Bi_k \rightarrow \infty, k = 1, 2;$$

$$\begin{cases} t_\tau = at_{xx}, \tau > 0, x \in (0, h) \\ t(x, 0) = t_0 \\ t(0, \tau) = \tilde{t}_0, t(h, \tau) = \tilde{t}_h \end{cases},$$

where α_0, α_h - are the heat transfer coefficients on the opposite surfaces of ES;

$\tilde{t}_0, \tilde{t}_h$ - are the specified temperatures of the external environments;

τ - time, [s];

a - is the thermal diffusivity, [m²/s];

λ - is the thermal conductivity, [W/m deg];

∇ - is the gradient, [1/m];.

The solution of the non-uniform, non-stationary, and asymmetric boundary value problem (1)-(4) under boundary conditions of the first kind ($\alpha_0 \rightarrow \infty, \alpha_h \rightarrow \infty$) by the Fourier method leads to the result:

$$\begin{aligned} w(x, \tau) &= \frac{2}{\pi} (t_0 - \tilde{t}_0) \sum_{n=1}^{\infty} \frac{\sin \frac{n\pi x}{h}}{n} e^{-\frac{n^2 \pi^2 a \tau}{h^2}} \\ &+ \frac{2}{\pi} (\tilde{t}_h - t_0) \sum_{n=1}^{\infty} (-1)^n \frac{\sin \frac{n\pi x}{h}}{n} \exp\left(-\frac{n^2 \pi^2 a \tau}{h^2}\right), \\ t(x, \tau) &= \tilde{t}_0 - (\tilde{t}_0 - \tilde{t}_h) \frac{x}{h} + w(x, \tau). \end{aligned}$$

If only one term $n=1$ of the series is taken into account:

$$w(x, \tau) \approx w_1 = \frac{2}{\pi} [(t_0 - \tilde{t}_0) - (\tilde{t}_0 - \tilde{t}_h)] e^{-\frac{\pi^2 a \tau}{h^2}} \sin \frac{\pi x}{h}$$

Or in dimensionless form

$$\Theta(\eta, Fo) = 1 - \eta + W_1(\eta, Fo)$$

where $\eta = \frac{x}{h}$, $Fo = \frac{a\tau}{h^2}$, $\Theta = \frac{t_0(x, \tau) - \tilde{t}_h}{\tilde{t}_0 - \tilde{t}_h}$,

$$W_1(\eta, Fo) = \frac{1}{\tilde{t}_0 - \tilde{t}_h} w_1(\eta, Fo)$$

Let's assume the following conditions for the problem:

We assume the wall thickness $h = 1$ meter to simplify the calculations. Thermal diffusivity of brick $a = 0.7$ m²/s, summation over (n) : Approximate calculation of the Fourier series up to 100 terms to achieve sufficient accuracy.

Let's write down the conditions for mathematical modeling of the physical process:

Initial moment $(x, 0) = t_0$, the temperature is constant throughout the wall.

Over time $\tau > 0$, the temperature begins to spread from the boundary surfaces to the center of the wall, creating a temperature gradient.

Over a long period of time $\tau \rightarrow \infty$, the temperature throughout the wall stabilizes, forming a linear gradient from the inner surface to the outer surface. The initial conditions no longer affect the ES, and the non-stationary process tends toward a quasi-steady-state regime.

Consider the following case, similar to the experimental ones described above, when:

The initial wall temperature $t(x, 0) = t_0$ is 0°C . The temperature on the inner surface: $t(x, \tau) = \tilde{t}_0$, $\tau = 0$ is $+18.1^\circ\text{C}$. Temperature on the outer surface $t(h, \tau) = \tilde{t}_h$, $\tau = 0$ is -28.1°C . In this case, the temperature distribution profile is shown in Figure 4.

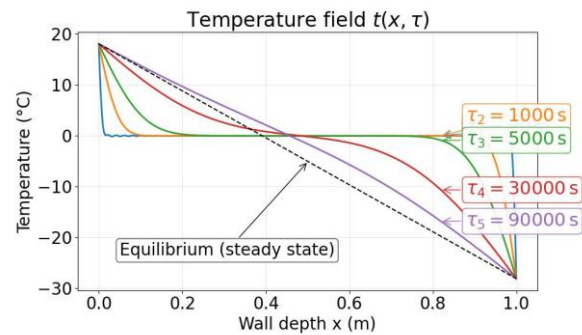


Fig. 4. Temperature profile of a brick wall at unsteady heat transfer:
(a) $t_0 = +18.1^\circ\text{C}$, $t_h = -28.1^\circ\text{C}$, (c) $t_{\text{wall}0} = 0^\circ\text{C}$

7. Analysis of Experimental Results and Their Numerical Modeling

The temperature field of enclosing temperatures in steady-state mode on the thermal resistance scale is shown in Figure 5. Regression lines (thin solid lines) were plotted for each experimental curve, showing a high degree of agreement with the experimental data (the square of the correlation coefficient is close

to 1), and equations were found in the form of second-degree polynomials. The maximum discrepancy between the calculated and experimental temperatures was: 1.8°C at a temperature in the cold compartment of the spacecraft at -32°C, 4.7°C at -11°C, and 5.2°C at -20°C.

Calculations were also performed using the program algorithm with the data presented in Table 2 (Figure 6).

For this calculation, numerical modeling of non-stationary thermal conductivity was used, specifically the explicit finite difference method, which sequentially updates the temperature at each spatial node based on heat flows from adjacent sections. The discontinuous properties of materials are also taken into account: since the wall consists of two different layers (brick and insulation), their thermal conductivity and heat capacity are defined as piecewise constants. At the boundaries between nodes, thermal conductivity is calculated as the harmonic mean to accurately transfer the heat flux across the material interface. To control the stability of the numerical scheme, the time step is chosen to be small enough to ensure the stability of the calculations, taking into account the maximum thermal diffusivity among the layers. An integral representation of thermal resistance is used instead of a physical coordinate across the wall thickness. The accumulated thermal resistance $Ro = \sum Ri$ from the inner surface is used to plot graphs, allowing for a clear display of the temperature field distribution, accounting for differences in the thermophysical properties of the brick. The steady-state temperature profile $t(x)$ at $\tau = 0$ is calculated separately, for which the heat flux is constant throughout the wall thickness, and is often used for comparison with non-stationary results. The solution domain is divided into a uniform grid across the wall thickness, and the heating/cooling process is modeled step-by-step in time at a given coordinate step (the thickness of the ES). These approaches allow for modeling and visualizing the heating or cooling dynamics of a multilayer ES from the initial state to a steady-state thermal regime.

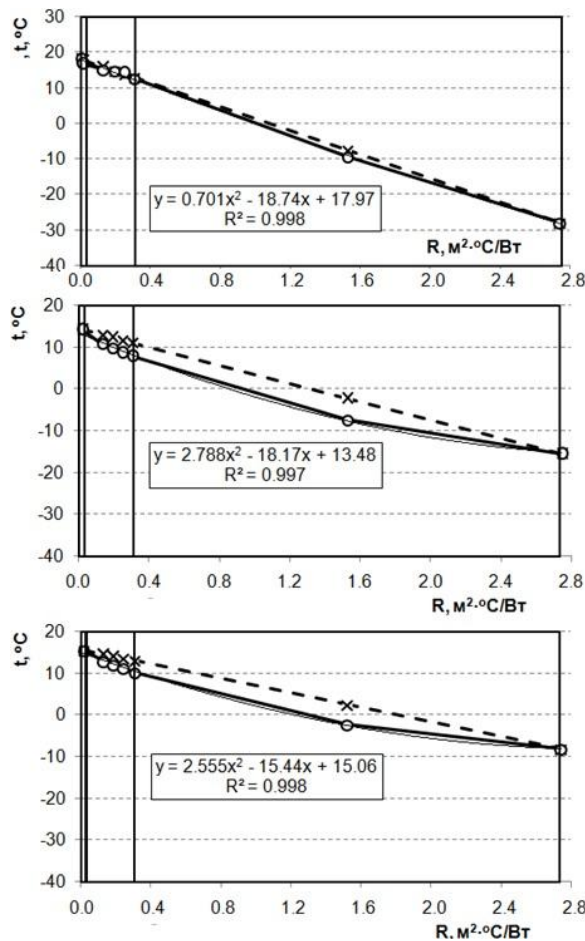


Fig. 5. Temperature profiles under different cold-chamber conditions (solid line – experiment, dashed – calculation):

(a) $t_o = -32^\circ\text{C}$, (b) $t_o = -20^\circ\text{C}$, (c) $t_o = -11^\circ\text{C}$

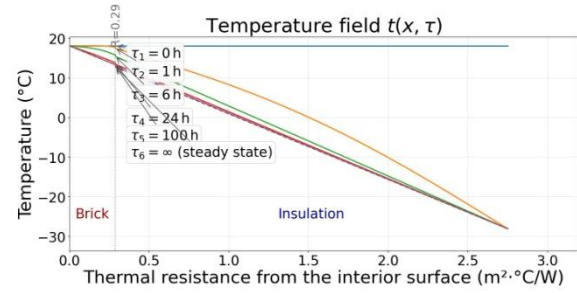


Fig. 6. Temperature profile of a brick wall with insulation at unsteady heat transfer:

(a) $t_o = +18.1^\circ\text{C}$, $t_h = -28.1^\circ\text{C}$, (c) $t_{\text{wall}o} = +18.1^\circ\text{C}$

8. Conclusions

These studies confirm that calculation methods for determining the thermal performance of building envelope structure, based on standards, often overestimate the energy efficiency of buildings. This is due to the underestimation of real-world operational factors: thermal bridges, installation defects, moisture accumulation in the insulation, and the dynamic nature of heat and mass transfer. Experimental data obtained in a climate chamber demonstrate significant discrepancies between theoretical and actual values of thermal resistance and thermal conductivity—in some cases, up to 25%.

The developed measurement data processing method, which combines thermography and dynamic approaches with numerical modeling of transient heat transfer, significantly improves the accuracy of assessing the actual thermal performance of structures. The use of hybrid methods for automated diagnostics and detection of hidden defects is particularly promising.

Thus, the transition to truly energy-efficient and sustainable construction requires the unified development of advanced materials, digital diagnostic methods, and dynamic models, using BIM technologies, quantum computers, and technologies that take into account the interrelationships between thermal and moisture exchange processes in enclosing structures at all stages of the life cycle of a building or structure or other multilayer structures, including techno-neural and electrical networks in the fields of power engineering, aerospace engineering, and other industries.

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Mathematical modeling of the hydrogen supply chain — an integrated approach for sustainable transport

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Abstract: This study proposes a mathematical model for design and optimization of a hydrogen supply chain, covering all stages of the life cycle - feedstocks, production, storage, distribution, end-use in the transport sector. The developed methodology integrates different hydrogen production technologies and takes into account environmental, economic and social impacts in order to identify the most efficient and sustainable configuration. The focus in this work falls on hydrogen production by steam reforming of methane and hydrogen production by electrolysis of water in hydrogen refueling stations. The mathematical model is formulated in terms of MILP programming and can be solved using the GAMS software product. The aim is to find an optimal balance between economic efficiency, environmental sustainability and social impact by using weighted coefficients (weights). The proposed concept provides a decision-making tool for planning hydrogen infrastructure in line with European decarbonization and sustainable transport goals.

Keywords: MILP, OPTIMIZATION, SUSTAINABLE, SUPPLY CHAIN, HYDROGEN

1. Introduction

Energy conservation has emerged as one of the key challenges of the modern world. This is due to the gradual but inevitable depletion of natural feedstocks, as well as the complex economic, political and social situation in different regions, also affecting ecosystems. These circumstances have prompted the scientific community to seek solutions to global problems, such as the development of alternative energy sources and the promotion of sustainable use of energy carriers. Recently, the integration of hydrogen technologies has been seen as a key factor in achieving carbon neutrality [1] and requires cooperation between scientific institutions, industry and political structures [2]. Especially in the transport sector, the use of hydrogen as a fuel is essential for reducing GHG emissions and increasing sustainability, and strategic planning of hydrogen supply chain can ensure the long-term stability of energy systems. Hydrogen technologies are expected to play a crucial role in the transformation towards a sustainable energy future in terms of transport. Over the past few years, the fuel and energy systems in transportation have been evolving from conventional fossil fuels to renewable energy sources [3]. However, there are problems with regard to high cost, inconsistent supply, and reliability [4].

Although atomic hydrogen is the most abundant chemical element in the universe [5], it is very rarely found in its pure form. Hydrogen can be produced through various technological processes, such as water electrolysis or steam methane reforming. The choice of hydrogen production method largely determines its environmental impact, energy efficiency, and economic feasibility. Among the most widely applied technologies, water electrolysis and steam methane reforming (SMR) differ significantly in terms of carbon footprint and energy input. Electrolysis, when powered by renewable energy sources, enables the production of nearly carbon-free hydrogen, making it one of the most promising pathways for achieving climate neutrality. Conversely, SMR remains the dominant industrial method due to its high efficiency and lower production costs, although it is associated with considerable CO₂ emissions. Other emerging technologies, such as biomass gasification, photoelectrochemical water splitting, and thermochemical cycles, are being investigated as potential alternatives that could enhance sustainability and reduce reliance on fossil fuels. The integration of these production pathways within a unified hydrogen economy requires comprehensive assessment of technical performance, cost efficiency, and environmental compatibility to ensure a balanced transition toward sustainable energy systems.

Depending on the technological production methods, hydrogen is classified into several color categories [6]. These colors categories are in turn divided into standard and innovative. The standard colors of hydrogen include “green hydrogen” - produced via electrolysis using renewable energy sources; “gray hydrogen” - produced via steam methane reforming (SMR), a process that also

generates carbon dioxide, which is ultimately released into the atmosphere; “blue hydrogen” - produced from fossil fuels, but unlike gray hydrogen, its production is associated with the capture and storage of greenhouse gases in underground storage sites; “black/brown hydrogen” - produced from coal. The innovative color categories of hydrogen include pink, gold, yellow, turquoise and white.

The use of hydrogen as an energy carrier has its advantages and disadvantages [7]. Some of the main positive properties of hydrogen are high gravimetric energy density, decarbonization potential, flexible energy storage, good integration in the existing energy infrastructure [8], diversification of energy sources and reduced dependence on fossil fuels [9]. From another perspective, hydrogen also has disadvantages, such as low volumetric energy density, high production costs [10], high energy losses as a result of compression and transportation, stringent safety requirements.

Currently, the implementation of hydrogen in the energy infrastructure around the world remains expensive and difficult. Although there is an increase in the number of hydrogens refueling stations [11] (mainly in Japan, South Korea, the USA and parts of the EU), the design of sustainable supply chains is still in its early stages. In order to enable the widespread adoption of hydrogen technology in the transport sector, it is necessary to develop a stable and sustainable supply chain. Such a hydrogen infrastructure must ensure the three pillars of sustainability – environmental, economic and social.

The scientific community has increasingly focused on developments on issues related to the hydrogen supply chain. Various methodologies and mathematical models have been proposed, with the studies most often emphasizing economic efficiency, while social and environmental aspects remain secondary. In addition, there is a lack of spatio-temporal integration between the stages of production, storage, transport and refueling. It is in this context that our study is positioned - developing a unified optimization framework that equally takes into account economic, environmental and social criteria.

The focus of the present work falls on green hydrogen – produced by electrolysis of water and using renewable energy sources and gray hydrogen, produced by steam reforming of methane. These two technologies represent the most established and contrasting hydrogen production pathways—SMR for its economic efficiency and maturity, and electrolysis for its environmental sustainability and renewable potential. Both production methods are integrated into a combined resource security chain. The present study proposes a MILP-based approach for sustainable design of an integrated superstructure of a supply chain. Optimization problem has been formulated and solved either at in terms of economic, social and environmental sustainability. The purpose of the defined mathematical model is to obtain optimal operating conditions of the considered an integrated supply chain. The proposed approach has

been solved using GAMS software, and the results can serve as a decision-support tool.

2. Formulation of the optimization problem

This study presents an integrated superstructure of a supply chain of hydrogen production via various technologies. The focus here is on hydrogen produced via steam methane reforming (SMR), as well as via electrolysis using renewable energy. The proposed superstructure views the supply chain system as a whole. It comprises feedstocks, production, storage, end user's areas and is represented in Fig. 1.

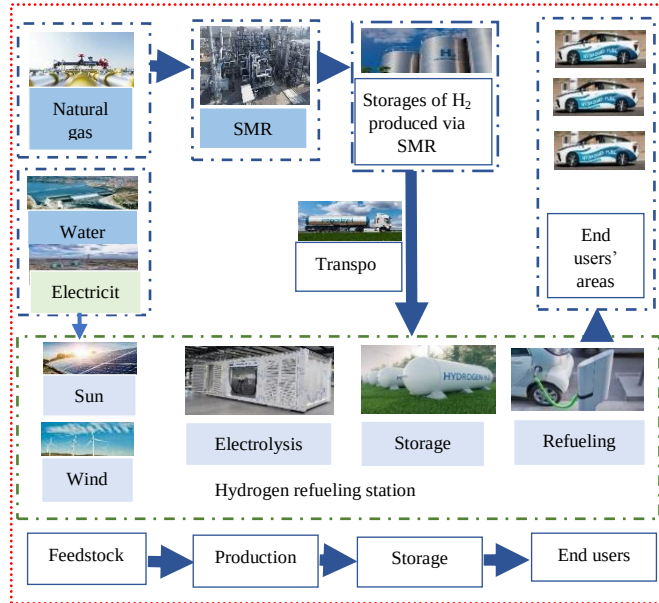


Fig. 1 An integrated superstructure of a supply chain

The problem considered in this paper can be formulated as follows Table 1:

Table 1: Problem statement

Given are:	Determine the optimal parameters of the supply chain as:
the location and production capacity of plants for hydrogen production via SMR	size, capacity and location of refueling stations
the potential location and capacity of storage facilities	size, capacity and location of hydrogen storage facilities
the potential locations of charging stations and their production capacity	the transport delivery scheme
the technologies for production of hydrogen via SMR and electrolysis	the total environmental impact as a result of the operation of all system during its operation
the price of raw materials (water, electricity and natural gas) and selling price of hydrogen	the total social impact as a result of the operation of all system during its operation
The type of transport for hydrogen delivery and transport costs	the total economic impact as a result of the operation of all system during its operation
greenhouse gas emissions for each stage of the life cycle and carbon tax	
government incentives for hydrogen consumption and production	
maintenance and operation costs of charging stations and labor cost	
demand at regions	

The problem is formulated as an optimization procedure in terms of mixed integer linear programming. The aim is to identify such decision variables that, subject to the system of constraints, minimize the objective function Z . The constraints guaranteeing the

performance of the task are linear functions with respect to all independent variables. The model aims to achieve an optimal balance between environmental sustainability, economic efficiency, and social impact when designing the hydrogen supply chain for the transportation sector.

The presented optimization procedure, which generates the mathematical model of a sustainable supply chain for hydrogen production for transport sector, is accompanied by preliminary collection and processing of the necessary data. In this case, two different technologies for hydrogen production are considered. Specifically, hydrogen production by steam methane reforming (SMR) and hydrogen production by electrolysis in hydrogen refueling stations (HRS) powered by renewable energy sources.

2.1. Input data for the test example

This part of the paper presents some of the necessary data.

• Territorial distribution

According to Geodesy, Cartography and Cadaster Agency [12] under the Ministry of Regional Development and Public Works, the total area of the Republic of Bulgaria is 111,002 km². In the case under consideration, Bulgaria is territorially divided into 28 administrative-territorial units (Fig.2).

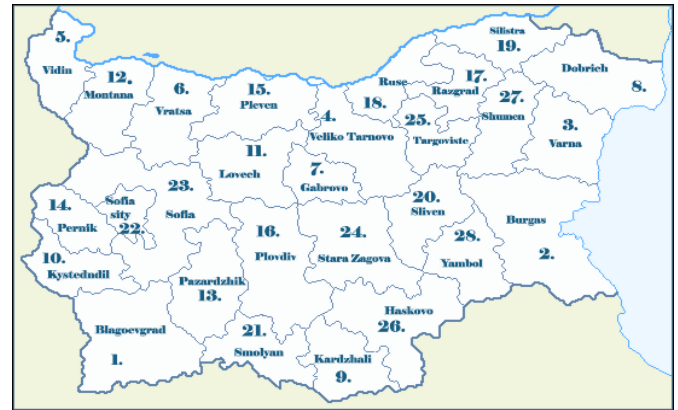


Fig. 2 Administrative - territorial units of Bulgaria

The hydrogen supply chain consists of 28 potential storage sites for hydrogen produced via steam reforming of methane, 28 potential sites for hydrogen production via electrolysis in Hydrogen Refueling Stations (HRS), 28 potential customer areas and 3 areas for hydrogen production by steam reforming. It is possible to build more than one Hydrogen Refueling Station in individual areas.

• Data on the actual delivery distance between

The distances in kilometers between regions in Bulgaria for the purposes of this study were taken from the Ministry of Regional Development and Public Works, Road Infrastructure Agency [13] for each mode of transport.

• Data on the type of transport for hydrogen delivery

According to the Agreement on the International Carriage of Dangerous Goods by Road (ADR), mandatory for the EU, including Bulgaria [14], gaseous hydrogen (flammable gas Class 2.1.) must be transported in special tanks or cylinders.

• Data on transport cost

It is assumed that all transportation will be carried out by land roads. Transportation costs include three main components: loading and unloading costs, time-dependent costs, and costs dependent on the distance between regions.

• Data on environmental parameters

Carbon emissions [kg CO₂-eq per kg H₂ per km] emitted during hydrogen transport are calculated taking into account the

average fuel consumption for the respective type of transport, the emission factor of the fuel (diesel) and the capacity of the trucks. The emission factor for the combustion of petroleum diesel (direct emissions - tank-to-wheel), the emission factor for the production of diesel, the emission factor for the entire life cycle of petroleum diesel, including production (gray emissions - well-to-wheel) are taken into account.

- *Capital Expenditure Data*

The capital costs of individual structures themselves represent fixed and variable capital costs.

- *Data on the type of hydrogen refueling stations*

For the purposes of this study, hydrogen refueling stations intended only for vehicles that meet the requirements of Regulation (EC) No 79/2009 of the European Parliament and of the Council on type-approval of hydrogen-powered motor vehicles are considered.

- *Data on demand*

Hydrogen market demand data presents a forecast of the market demand for hydrogen as an automotive fuel based on the population size of a given area. Calculations have been made for a scenario where 0.5% of cars would be hydrogen-powered, given the available infrastructure and incentives.

- *Data on monetary parameters in hydrogen production by electrolysis*

It is assumed that the envisaged fixed premium for the production of green hydrogen is between €0.37 and €0.48 per kg of H₂, with a ceiling of €4.5/kg. (\$0.43 - \$0.56 with a ceiling of \$5.24 per kilogram of hydrogen) [15].

- *Data on time intervals*

According to the strategic legislative package "Fit for 55" [16] developed by the European Commission, the rules for integrated and transparent network planning across the EU according to the "energy efficiency first" principle and with a future-oriented approach, gas and hydrogen network operators will have to prepare a 10-year EU network development plan. For the purposes of this task, a 5-year time frame is considered. The entire time horizon H is divided into a set of discrete time intervals t. This time interval is divided into several equal time subintervals t={0,1,2,...,T}, each of which lasts ∇t .

2.2. Environmental assessment model

The environmental assessment model of the integrated hydrogen supply chain is represented as the total greenhouse gas emissions generated over the whole live. They are converted into carbon credits multiplied by the price of carbon emissions on the market.

$$E_t = EProd_t + EStor_t + EOwn_t + ETrans_t + EFossil_t, \forall t \quad (1)$$

Where:

E_t - The total environmental impact of the Hydrogen Supply Chain operation over its entire life cycle, [kgCO_{2eq}/y];

$EProd_t$ - Greenhouse gas emissions released during hydrogen production via SMR, [kgCO_{2eq}/y];

$EStor_t$ - Greenhouse gas emissions released during hydrogen storage, [kgCO_{2eq}/y];

$EOwn_t$ - Greenhouse gas emissions released during hydrogen production via the electrolysis process, [kgCO_{2eq}/y].

$ETrans_t$ - Greenhouse gas emissions released during the transportation of hydrogen (Tank-to-Well), [kgCO_{2eq}/y];

$EFossil_t$ - Greenhouse gas emissions released during from the production of diesel fuel, associated with diesel (Well-to-Tank), [kgCO_{2eq}/y];

2.3. Social assessment model

The social assessment model of the integrated hydrogen supply chain is represented as the total labor costs are calculated for each stage — production, storage, transport, and local production — as a function of the amount of hydrogen processed and the labor intensity of the respective technology.

$$L_t = LProd_t + LStor_t + LOwn_t + LTrans_t, \forall t \quad (2)$$

Where:

L_t - The total social impact of the Hydrogen Supply Chain operation over its entire life cycle, [\$/y];

$LProd_t$ - Labor costs in hydrogen production via SMR, [\$/y];

$LStor_t$ - Labor costs for hydrogen storage, [\$/y];

$EOwn_t$ - Labor costs in hydrogen production via the electrolysis process, [\$/y];

$ETrans_t$ - Labor costs for hydrogen transportation, [\$/y];

2.4. Economic assessment model

For definition of the economic assessment model of the supply chain operation the annual operating costs are used. The economic criterion includes the total investment costs, both operational costs (energy, raw materials, transport, labor) and investment costs for building the infrastructure. The model also includes government subsidies and a carbon tax, which affect the net costs of the system for the planned time period. They define for each time interval t ∇t as:

$$TC_t = TCProd_t + TCStor_t + TCOwn_t + TCTrans_t + TCOwn_t^{inv} + TCStor_t^{inv} + CarbTax_t - Sub_t, \forall t \quad (3)$$

Where:

TC_t - The total economic impact of the Hydrogen Supply Chain operation over its entire life cycle, [\$/y];

$TCProd_t$ - Operating expenditure (OPEX) for hydrogen production via SMR, [\$/y];

$TCStor_t$ - Operating expenditure (OPEX) for hydrogen storage, [\$/y];

$TCOwn_t$ - Operating expenditure (OPEX) for hydrogen production via the electrolysis process, [\$/y];

$TCTrans_t$ - Transportation expenditure, [\$/y];

$TCOwn_t^{inv}$ - Capital expenditure (CAPEX) for HRS, [\$/y];

$TCStor_t^{inv}$ - Capital expenditure (CAPEX) for Storages, [\$/y];

$CarbTax_t$ - Carbon tax, [\$/y];

Sub_t - Government incentives, [\$/y];

2.5. Constraints

The constraints that guarantee the completion of the task are linear functions of all independent variables. The constraints that guarantee the completion of the task are linear functions of all independent variables. These constraints are related to the capacity of the facilities, the material balance, flows admissibility, needs of hydrogen as fuel, logistical and transportation constraints and others. The planning horizon is set to 5 years.

2.6. Objective function

The optimization problem for determining the optimal location of the plants in the regions and their parameters is formulated as:

$$Z = \alpha \cdot TC_t + \beta \cdot E_t + \gamma \cdot L_t \quad (4)$$

$$\text{Find: } X_t [\text{Decision variables}] \text{ MINIMIZE } \{Z(X_t)\} \rightarrow \\ (\text{Eq. 4}) \text{ s. t. : } \{\text{Constraints}\} \quad \dots\dots (5)$$

Where

α, β, γ – weighting factors that determine the priority of each criterion.

The objective function Z aims to minimize the overall value derived from a weighted combination of economic, environmental, and social factors.

The optimization problem can be solved using the GAMS software, which enables comprehensive and intelligent decision-making.

The results obtained from the developed methodology will be presented and discussed in a forthcoming paper. Further research will elaborate on the implementation and analysis of the proposed approach.

In addition, by adjusting the required data, the proposed model can be adapted to various regions.

4. Conclusion

The study proposes an integrated approach for design of hydrogen supply chain. The proposed mathematical model is formulated in terms of MILP. Sustainability is considered from the perspective of economic, environmental and social factors. It is proposed an integrated superstructure of a supply chain including various technologies for hydrogen production and considering the supply chain as a whole from feedstock to end users. The proposed task is solved using the GAMS software platform, which can serve as a decision-support tool.

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Reliability Criteria for the Working Elements of Robotic Systems

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Abstract. The article presents the rationale for an algorithm describing the interaction of random peak load parameters and strength parameters used in defining the reliability criteria for the working elements of robotic systems. The assessment method is founded upon finding the probability of attaining a dangerous state during the realization of an extreme random process within the calculated operational time interval. To facilitate this analysis, the random parameters of the load and the strength of the machine's working element are represented as functional dependencies of the generalized load and generalized strength on time.

KEYWORDS: SAFETY MARGIN, RELIABILITY, CRITICAL ELEMENTS OF AGRICULTURAL MACHINERY, STATISTICAL APPROACH, OVERLOAD.

Introduction

The structural parameter calculations for parts and working elements of robotic systems employed in agricultural production must fundamentally ensure their strength and durability during the effective performance of their specified technological functions. The successful operability of such systems, when subjected to various types of working loads, is dependent on a confluence of factors, including specific technological parameters of the production process, ambient environmental conditions, the physical properties of the materials used, and the features of the structural design [1-3]. It is essential that the challenge of guaranteeing strength and long life under the influence of working loads—which vary significantly in magnitude, shape, and periodicity—is addressed comprehensively during the calculation and projection stages of design [4-6]. Failure to account for dynamic effects can be detrimental, as non-stationary loads, excessive vibrations, and short-term overloads possess the capacity to substantially diminish the quality and overall performance of the constructed machine [7].

Consequently, establishing robust reliability criteria for the working elements of robotic systems employed in agricultural manufacturing remains one of the priority tasks in contemporary mechanical engineering [8, 9]. To effectively develop robotic systems and complexes possessing higher inherent reliability, it is necessary to consider and implement new calculation principles. This includes advancing methods for theoretical research that specifically address operational conditions characterized by the presence of short-term overloads. The nature of agricultural work, involving high levels of stochastic environmental factors (such as impacts and rapid load fluctuations), dictates that models focusing on instantaneous failure criteria are paramount for design accuracy.

Results and Discussion

This specifically investigates the calculation of working elements within robotic systems that operate under the influence of short-term, non-stationary loads characterized by a high level of intensity. It is important to note that, under these loading conditions, the analysis typically excludes the consideration of cumulative damage accumulation, such as fatigue or wear. Instead, the objective is centered on determining the probability of the structure reaching a dangerous state at least once during the realization of an extreme random process over the calculated operational time interval T .

To address this challenge, the random parameters governing the load and the strength of the working element are mathematically expressed as functional dependencies of time t . The calculated random parameters of the machine's working elements are separated into two distinct groups. Generalized strength $\tilde{R}(t)$: these parameters relate directly to the intrinsic properties of the working elements' structure. Generalized load $\tilde{F}(t)$: these parameters represent the forces generated in the working elements resulting from the externally acting loads.

In operational circumstances, both the generalized load $\tilde{R}(t)$ and the generalized strength $\tilde{F}(t)$ constitute random functions of time t . Therefore, the research task is reduced to analyzing the interaction between the functions $\tilde{F}(t)$ and $\tilde{R}(t)$ over the calculated operational time interval, $T = T_t$.

The failure of a machine's working element during the period T is mathematically defined when the magnitude of the load exceeds the capacity of the strength:

$$\tilde{F}(t) > \tilde{R}(t). \quad (1)$$

To facilitate probabilistic analysis, the random function of the safety margin, $\tilde{S}(t)$, is introduced. This function represents the difference between the available strength and the acting load:

$$\tilde{S}(t) = \tilde{R}(t) - \tilde{F}(t). \quad (2)$$

In the context of this definition, failure is precisely defined as the function $\tilde{S}(t)$ obtaining negative values:

$$\tilde{S}(t) < 0. \quad (3)$$

Knowledge of the statistical characteristics of the independent random functions $\tilde{F}(t)$ and $\tilde{R}(t)$ —specifically their mathematical expectations $m_F(t)$, $m_R(t)$ and correlation functions $K_F(t_1, t_2)$, $K_R(t_1, t_2)$ —permits the determination of the characteristics of the random safety margin function $\tilde{S}(t)$:

- Mathematical expectation: $m_S(t) = m_R(t) - m_F(t)$;
- Correlation function. Assuming the absence of a mutual correlation link between load and strength $K_{FR}(t_1, t_2) = 0$, the correlation function of the safety margin is given:
 $K_S(t_1, t_2) = K_R(t_1, t_2) + K_F(t_1, t_2)$;
- Dispersion: $D_S(t) = K_S(t) = D_R(t) + D_F(t)$.

The assumption of zero mutual correlation is a practical simplification often adopted in reliability models where the variability originating from manufacturing processes (affecting R_t) is considered statistically independent from the variability originating from the operating environment (affecting F_t). These initial statistical definitions enable designers to quantify the inherent risk by combining structural tolerances with expected operational extremes.

Given the premise that the probability of failure caused by an overload event—and the resultant loss of reliability of the machine elements sufficiently small, a Poisson-type stochastic model is adopted for the analysis. This model allows for the determination of the intensity of disturbances (failure rate) and the subsequent reliability function associated with the safety margin $\tilde{S}(t)$.

Since the critical transition (the disturbance) occurs when $\tilde{S}(t)$ moves into the negative range, the average number of negative values (crossings below the zero level) per unit time ($\bar{U}^-(0)$) is derived using the following integral expression:

$$\bar{U}^-(0) = - \int_{-\infty}^0 \dot{\tilde{S}} \cdot p(0, \dot{\tilde{S}}) d\dot{\tilde{S}}, \quad (4)$$

where $p(0, \dot{\tilde{S}})$ is the joint probability density of the safety margin function $\tilde{S}(t)$ and its time derivative, $\dot{\tilde{S}}(t)$, at every moment of time t .

The derivative $\dot{\tilde{S}}(t)$ is mathematically defined as the speed of change of the safety margin:

$$\dot{\tilde{S}}(t) = \frac{d\tilde{S}(t)}{dt} = \frac{d\tilde{R}(t)}{dt} - \frac{d\tilde{F}(t)}{dt}. \quad (5)$$

The negative sign preceding the integral in expression (4) is essential, as it denotes a negative speed ($\dot{\tilde{S}} < 0$), which corresponds precisely to the dynamic condition of the function moving downward past the zero level and into the failure region.

For the practical calculation of instantaneous failure intensity within the operational interval, the generalized strength $\tilde{R}(t)$ of the

structural element is conventionally considered a random constant value, denoted as $\tilde{R}(t) = \tilde{R}$.

Under this simplifying condition, the safety margin expression becomes:

$$\tilde{S}(t) = \tilde{R} - \tilde{F}(t). \quad (6)$$

Consequently, the time derivative simplifies significantly, as the derivative of the constant strength component is zero ($\frac{d\tilde{R}}{dt} = 0$):

$$\dot{\tilde{S}}(t) = \frac{d\tilde{R}}{dt} - \frac{d\tilde{F}(t)}{dt} = -\dot{\tilde{F}}(t). \quad (7)$$

This means that the speed of change of the safety margin function is entirely determined by the speed of change of the generalized load function. This deterministic relationship between $\tilde{S}(t)$ and $\dot{\tilde{F}}(t)$ allows for the integration limits and variables in the failure intensity calculation to be transformed:

$$\int_{-\infty}^0 \dot{S} \cdot p_S(\dot{S}) d\dot{S} = \int_{-\infty}^0 \dot{F} \cdot p_F(\dot{F}) d\dot{F}. \quad (8)$$

Therefore, the final intensity of failures $\tilde{U}^-(0)$ is derived by the expression:

$$\tilde{U}^-(0) = -p_S(0) \int_{-\infty}^0 \dot{F} \cdot p_F(\dot{F}) d\dot{F}, \quad (9)$$

where $p_S(0)$ and $p_S(\dot{S})$ are the probability densities of the safety margin function and the load function and its derivative, respectively, at time t .

The Reliability Function $P(T)$, which represents the probability of failure-free operation of the working element as an individual object over the operation time T (considering both the object's structural features and the acting loads), is determined by integrating the intensity of failures over the operational period:

$$P(T) = [1 - H_S(0|R)] \exp \left[- \int_0^T \tilde{U}(0) dt \right]. \quad (10)$$

In this equation, $H_S(0|R)$ is defined as the conditional probability of structure failure at the initial time $t = 0$, accounting for potential initial defects or deficiencies.

These mathematical dependencies (1) – (10) are directly applicable to mechanical systems whose reliability is determined primarily by the reliability of the single, most heavily loaded working element. For complex multi-element systems, the total reliability function must necessarily rely on the aggregated reliability of all its constituent parts.

Conclusions

The presented detailed the interaction between random peak parameters of stochastic loading and the corresponding strength parameters of critical working elements within robotic mechanical systems. This methodology effectively represented these critical parameters as functional dependencies of generalized load $\tilde{F}(t)$ and generalized strength $\tilde{R}(t)$ on time.

The primary methodological advancement lies in the ability to assess the reliability of a system element by integrating the probabilistic aspects of the distribution of these dependencies, specifically under the influence of short-term overloads. By applying crossing theory to the safety margin distribution, the model provides a quantitative framework for assessing dynamic failure risk. This probabilistic approach, which moves beyond deterministic comparisons, significantly enhances the accuracy of calculations utilized for reliability prediction and, consequently, leads to a meaningful increase in the operational life (resource) of the machinery.

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Mathematical modelling of the lactic acid production from agro-industrial waste materials

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Abstract: Various agro-industrial by-products, such as distillers dried grains with solubles (DDGS), spent coffee grounds (SCG), and cheese whey, have promising potential as suitable substrates for second-generation lactic acid production.

The present study explores the potential of two *Lactiplantibacillus plantarum* strains—*L. plantarum* f53 and *L. plantarum* 2HS—for the efficient production of LA from the above-mentioned agro-industrial waste materials. Their comparable efficiency to pure lactose as a substrate suggests that these wastes can serve as sustainable, low-cost raw materials for industrial-scale LA production.

A mathematical model of the fermentation process was composed. The model includes differential equations describing cell growth, substrate consumption, and product formation. The modified Gompertz equation and the Luedeking–Piret equation were used to describe cell growth and lactic acid production. The proposed model was tested and showed excellent agreement with experimental data, and the calculated parameter values were of the same magnitude for all cases.

1. Introduction

Lactic acid bacteria (LAB) are a diverse group of taxonomically distinct microorganisms, united by their ability to form lactic acid during the fermentation of various carbon sources. Lactic acid production from different agro-industrial waste materials by *Lactiplantibacillus plantarum* strains was studied. Distiller's dried grains with solubles (DDGS), spent coffee grounds (SCG), wood chips hydrolysates (WH), and cheese whey were used as substrates after pretreatment, and the results were compared with those with lactose as a carbon source. A mathematical model of the fermentation process includes a set of coupled differential equations describing cell growth, substrate consumption, and product formation. The mathematical model based on the Compertz and Luedeking – Piret equations was proposed and tested, showing very good agreement with experimental data.

2. Objective

The purpose of the present investigation was to model the lactic acid production by selected *Lactobacilli* strains capable of assimilating the sugars present in some waste materials, to study the kinetics, and to model the process of lactic acid production. The waste streams were dilute acid and enzyme hydrolysates from DDGS and SCG, cheese whey, and a by-product stream from the Kraft process of cellulose production from wood. A mathematical model of the fermentation process includes a set of coupled differential equations describing cell growth, substrate consumption, and product formation.

$$X(t) = X_0 + \frac{A}{1 + \exp\left[\frac{4\mu_{\max}}{A}(\lambda - t) + 2\right]}$$

$$\frac{dP}{dt} = \alpha \frac{dX}{dt} + \beta X$$

$$\frac{dS}{dt} = -\frac{1}{Y_{X/S}} \frac{dX}{dt} - \frac{1}{Y_{P/S}} \frac{dP}{dt} - m_s X$$

$$t = 0, P = P_0, S = S_0$$

3. Research methodologies

MATLAB 2025b software was used to solve the model equations describing the fermentation process. Initially, the parameters in the modified Gompertz model ($\mu_{\max}$, A , λ) are determined using experimental data for cell concentration and minimizing the least square's function Q_1 , being the sum of the squares of the differences between the measured biomass and that calculated from the model. The next step is to solve the model equations describing lactic acid formation and substrate consumption. To calculate the parameter values ($Y_{X/S}$, α , β , $Y_{P/S}$), our experimental data were used, minimizing the least square's function Q_2 , which is the sum of the squares of the differences between the calculated concentrations by the model and measured substrate and lactic acid concentrations.

$$Q_1(\mu_{\max}, A, \lambda) = \frac{1}{N} \sum_{j=1}^N (X_j - X_j^{\exp})^2 \rightarrow \min$$

$$Q_2(Y_{X/S}, Y_{P/S}, \alpha, \beta) = \frac{1}{N} \sum_{j=1}^N (S_j - S_j^{\exp})^2 + \sum_{j=1}^N (P_j - P_j^{\exp})^2 \rightarrow \min$$

In both functions, Q_1 and Q_2 , j are the experimental point numbers; X , S , and P are values of the biomass, substrate, and product concentration calculated by the model; $X^{\exp}$, $S^{\exp}$, and $P^{\exp}$ are experimental values; N is the experimental data number; and t_j ($j = 1 \dots N$) are the times in which the X , S , and P concentrations are measured.

4. Results and discussion

Table 1. Determined model parameter values

Strain	Model parameters										
	$\mu_{\max}$	A	λ	$Y_{X/S}$	$Y_{P/S}$	α	β	Q_1	Q_2	R_1^2	R_2^2
<i>L. plantarum</i> f53	1	0.813	14.531	13.866	0.276	2.573	7.022	0.009	0.1895	0.2837	0.9986
	2	0.472	13.985	12.569	0.156	2.361	5.142	0.010	0.0696	0.5467	0.9984
	3	0.394	13.427	13.492	0.157	5.407	12.564	0.009	0.0309	0.0219	0.9998
	4	1.174	12.623	24.249	0.580	4.493	3.470	0.029	0.1013	0.0335	0.9914
	5	0.490	12.864	15.504	0.313	2.312	7.156	0.008	0.1231	1.2410	0.9950
<i>L. plantarum</i> 2HS	1	0.385	14.583	10.922	0.280	2.393	7.025	0.011	0.215	0.2347	0.9973
	2	0.405	13.129	10.580	0.435	3.541	2.701	0.018	0.1505	0.9457	0.9989
	3	0.376	12.590	12.975	0.191	4.905	10.349	0.006	0.1326	0.0212	0.9912
	4	1.033	11.769	24.332	0.349	4.731	5.712	0.016	0.0421	0.0706	0.9866
	5	0.544	11.978	17.448	0.2488	1.122	7.592	0.006	0.0874	1.2025	0.9920

1—Lactose; 2—Whey; 3—SCG; 4—WH; 5—DDGS; $\mu_{\max}$ —maximum growth rate, h^{-1} ; A —the asymptotic level of biomass, g/L; λ —duration of the lag phase, h; $Y_{X/S}$ and $Y_{P/S}$ —yield coefficients for biomass on substrate and product on substrate, respectively, g/g; α [–] and β [h^{-1}]—growth associated constants for product formation and the non-growth-associated constant for product formation, h^{-1} ; Q_1 , Q_2 —target functions, R_1^2 , R_2^2 —coefficients of determination.

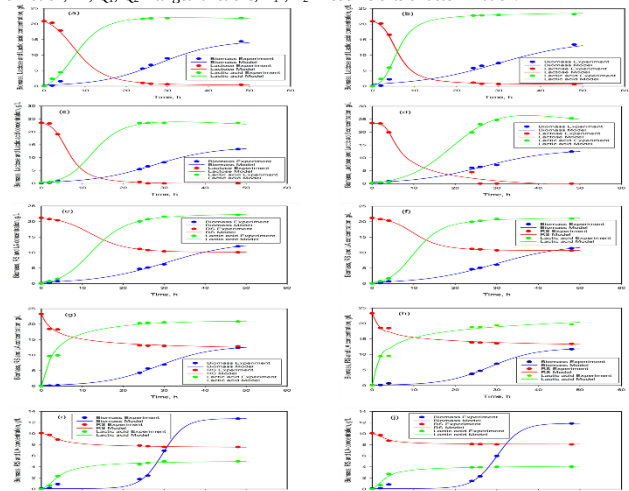


Fig 1. Experimental and model results for microbial growth, substrate consumption, and lactic acid production from different carbon sources

5. Conclusion

The possibility of using waste materials for lactic acid production was tested in the present study. Different raw materials were used – DDGS, SCG, wood hydrolysate, and whey. A mathematical model based on the modified Gompertz equation and the Luedeking–Piret equations was used to model experimental data, with excellent agreement. The parameter values calculated by the model for all cases were of the same magnitude.

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Mathematical modeling of innovative waste-free FGD process that combines absorption and adsorption

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One of the most dangerous air pollutants is sulfur dioxide. Its main source is the processes in which coal, oil and other fossil fuels, which have a high sulfur content, are burned. An innovative waste-free FGD process is proposed for decontamination of flue gases from SO_2 . It is an absorption-adsorption method based on the absorption of SO_2 in water with its simultaneous adsorption from the aqueous solution with a synthetic ion exchange resin. The regeneration of the adsorbent is carried out with a solution of NH_3 , with subsequent decomposition to obtain $(\text{NH}_4)_2\text{SO}_3$ with HNO_3 . The final products of the processes are pure, gaseous (liquefied) SO_2 and an aqueous solution of NH_4NO_3 . Sulfur dioxide has unlimited application in the chemical industry, and NH_4NO_3 is a commercial product - nitrogen fertilizer. In this sense, the new absorption-adsorption method represents a practically waste-free technology. The main element of this technology is a tray column, where the absorption-adsorption process takes place on the trays in an aqueous suspension of synthetic ion exchange resin (Fig.1.).

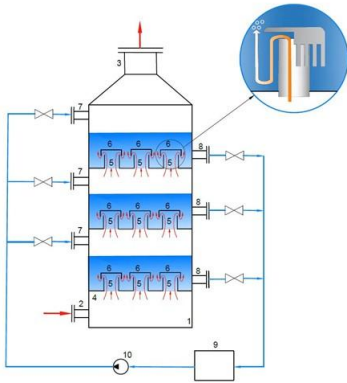


Fig.1. Scheme of the process

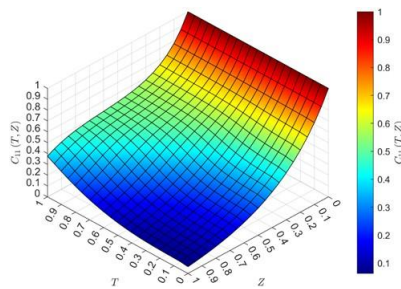


Fig.2. SO_2 (gas) concentration

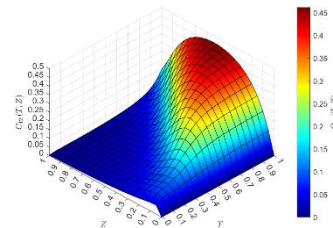


Fig.3. SO_2 (liquid) concentration

A convection-diffusion model for the specific process with generalized variables, axial and radial velocity components, has been developed. The equations of the average-concentration model and the convective-diffusion model have been solved. The parameters in the gas and liquid phases have been identified. For the mathematical description of the non-stationary absorption-adsorption process, a combination of physical absorption and chemical adsorption models is used (1)

$$\begin{aligned} \frac{\partial c_{11}^{(n)}}{\partial t} + u_1 \frac{\partial c_{11}^{(n)}}{\partial z} &= D_1 \frac{\partial^2 c_{11}^{(n)}}{\partial z^2} - k_0 (c_{11}^{(n)} - \chi c_{12}^{(n)}); \\ \frac{\partial c_{12}^{(n)}}{\partial t} + u_1 \frac{\partial c_{12}^{(n)}}{\partial z} &= D_1 \frac{\partial^2 c_{12}^{(n)}}{\partial z^2} + k_0 (c_{11}^{(n)} - \chi c_{12}^{(n)}) - k_1 (c_{12}^{(n)} - c_{13}^{(n)}); \\ \frac{dc_{13}^{(n)}}{dt} &= k_1 (c_{12}^{(n)} - c_{13}^{(n)}) - k c_{13}^{(n)} c_{23}^{(n)}, \quad \frac{dc_{23}^{(n)}}{dt} = -k c_{13}^{(n)} c_{23}^{(n)}; \\ t=0, \quad c_{11}^{(n)} &\equiv c_{11}^0, \quad c_{12}^{(n)} \equiv 0, \quad c_{13}^{(n)} \equiv 0, \quad c_{23}^{(n)} \equiv c_{23}^0; \\ z=0, \quad c_{11}^{(n)}(0) &\equiv c_{11}^{(n-1)}(l), \quad 0 \equiv \left(\frac{\partial c_{11}^{(n)}}{\partial z} \right)_{z=0}, \quad c_{11}^{(1)}(0) \equiv c_{11}^0, \quad 0 \equiv \left(\frac{\partial c_{12}^{(n)}}{\partial z} \right)_{z=0}; \\ z=l, \quad 0 &\equiv \left(\frac{\partial c_{12}^{(n)}}{\partial z} \right)_{z=l}. \end{aligned}$$

An experimental installation for the processes has been designed and built up. Experiments for the kinetic of the processes are carried on. The results of the mathematical modeling are in a good agreement with the experimental data. Fig.2. and Fig.3 represent the distribution of the SO_2 concentration with time and column height in the gas and the liquid phase respectively.

Key words: SO_2 , convection-diffusion model, absorption, adsorption, ionexchange resins,

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Modeling quantum correlations in donor-acceptor transport processes of biomolecules

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Abstract: A quantum model of excitation transfer from a donor molecule to an acceptor molecule through a biomolecule represented by a quasi-one-dimensional molecular chain is proposed. The sites of the chain correspond to the structural elements of biomolecules, such as amino acid residues linked into the chain by peptide bonds in proteins or nucleotides in RNA and DNA. Particular attention is paid to the emergence of quantum entanglement between the donor and acceptor molecules as the specific type of quantum correlations, which provides an intramolecular quantum channel for information transmission.

Keywords: TRANSPORT PROCESSES, BIOMOLECULES, QUANTUM ENTANGLEMENT, LOGARITHMIC NEGOTIVITY

1. Introduction

Transport processes of energy and charge in biomolecules, such as proteins, RNA and DNA, play an important role in cellular vital functioning. For example, it is believed that protein molecules are the mediators of transfer of energy generated in the hydrolysis of triphosphate (ATP) for diverse biological processes such as photochemical reactions, cross-membrane ion transfer and muscle contraction. Such processes, as has been shown, cannot be described within the framework of classical physics, but a quantum mechanical approach is required [1]. Moreover, the description of transport processes in highly molecular structures at the quantum mechanical level makes it possible to consider also the question of quantum correlations arising in such systems [2, 3]. It is currently believed that quantum correlations and entanglement between the electronic states of nucleic acids in DNA are responsible, in particular, for the processes of its repair and replication (see, e.g., [4]). However, experimental verification of quantum entanglement in biomolecules is very difficult due to the structural complexity of these molecules. In this sense, the use of donor and acceptor molecules attached to specific sites of a biomolecule to provide excitation transport can be used as detectors to register quantum correlations that might arise between these sites of the biomolecule.

2. Model Hamiltonian of a Biomolecule with Attached Donor and Acceptor Molecules

We consider a model of a biomolecule as a quasi 1D periodic polymer chain of N structural elements (or sites) located at a distance of R (the primary structure). As the structural elements of biomolecules, one can consider amino acid residues linked into the chain by peptide bonds in proteins or nucleotides in RNA and DNA. The donor and acceptor molecules are assumed to be attached to the molecular chain (MC) at the certain sites (e.g., n_1 and n_2). Then the Hamiltonian of such a composite system has the form of the sum of the following Hamiltonians:

$$\hat{H} = \hat{H}_{MC} + \hat{H}_D + \hat{H}_A + \hat{H}_{D-MC} + \hat{H}_{A-MC}, \quad (1)$$

where

$$\hat{H}_{MC} = \sum_{n=1}^N \left[\hbar \Delta \hat{a}_n^\dagger \hat{a}_n - \frac{\hbar L}{2} (\hat{a}_{n+1}^\dagger \hat{a}_n + \hat{a}_{n-1}^\dagger \hat{a}_n) \right] \quad (2)$$

describes intramolecular excitation states in MC with the energy $\hbar \Delta$ and $\hbar L/2$ is the energy of intermolecular interactions between two neighboring sites, $\hat{a}_n^\dagger$ being the excitation creation operator on the n -th lattice site,

$$\hat{H}_D = \hbar \varepsilon_D \hat{D}^\dagger \hat{D}, \quad \hat{H}_A = \hbar \varepsilon_A \hat{A}^\dagger \hat{A} \quad (3)$$

correspond to the donor and acceptor molecules with the energies $\hbar \varepsilon_D$, $\hbar \varepsilon_A$, and $\hat{D}^\dagger$, $\hat{A}^\dagger$ are their creation operators, which attached to n_1 and n_2 sites of the molecular chain in a form of

$$\hat{H}_{D-MC} = \hbar \delta_D (\hat{a}_{n_1}^\dagger \hat{D} + \hat{D}^\dagger \hat{a}_{n_1}), \quad \hat{H}_{A-MC} = \hbar \delta_A (\hat{a}_{n_2}^\dagger \hat{A} + \hat{A}^\dagger \hat{a}_{n_2}) \quad (4)$$

with the coupling energies $\hbar \delta_D$ and $\hbar \delta_A$.

Applying to the site operators $\hat{a}_n$ the following transformation

$$\hat{a}_n = \frac{1}{\sqrt{N}} \sum_{k=-\pi/R}^{\pi/R} \hat{a}_k \cdot \exp\{iknR\}, \quad (5)$$

where the vector $k = 2\pi v/(NR)$, $v = -N/2 + 1, -N/2 + 2, \dots, 0, \dots, N/2 - 1, N/2$, takes N discrete values in the interval $-\pi/R < k \leq \pi/R$, Hamiltonian (1) takes the form in the k -representation

$$\hat{H} = \sum_{k=-\pi/R}^{\pi/R} [\hbar \omega_k \hat{a}_k^\dagger \hat{a}_k + \hbar V_D(k) \hat{a}_k^\dagger \hat{D} + \hbar V_D^*(k) \hat{D}^\dagger \hat{a}_k + \hbar V_A(k) \hat{a}_k^\dagger \hat{A} + \hbar V_A^*(k) \hat{A}^\dagger \hat{a}_k + \hbar \varepsilon_D \hat{D}^\dagger \hat{D} + \hbar \varepsilon_A \hat{A}^\dagger \hat{A}] \quad (6)$$

with

$$\omega_k = \Delta - L \cdot \cos(kR), \quad (7)$$

$$V_D(k) = \frac{\delta_D}{\sqrt{N}} \exp\{-ikn_1R\}, \quad V_A(k) = \frac{\delta_A}{\sqrt{N}} \exp\{-ikn_2R\}. \quad (8)$$

In order to describe the dynamics of such a system, we represent the wave function for a single-excitation state in the form

$$|\psi(t)\rangle = [u_D(t) \hat{D}^\dagger + u_A(t) \hat{A}^\dagger + \sum_{k=-\pi/R}^{\pi/R} u_k(t) \hat{a}_k^\dagger] |0\rangle \quad (9)$$

with the normalization condition for the amplitudes

$$|u_D(t)|^2 + |u_A(t)|^2 + \sum_{k=-\pi/R}^{\pi/R} |u_k(t)|^2 = 1. \quad (10)$$

The amplitudes are found from the Schrödinger equation

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = \hat{H} |\psi(t)\rangle, \quad (11)$$

which leads to the following system of differential equations

$$\begin{aligned} \frac{du_D(t)}{dt} &= -i \left[\varepsilon_D u_D(t) + \sum_{k=-\pi/R}^{\pi/R} V_D(k) u_k(t) \right], \\ \frac{du_A(t)}{dt} &= -i \left[\varepsilon_A u_A(t) + \sum_{k=-\pi/R}^{\pi/R} V_A(k) u_k(t) \right], \\ \frac{du_k(t)}{dt} &= -i [\omega_k u_k(t) + V_D^*(k) u_D(t) + V_A^*(k) u_A(t)], \end{aligned} \quad (12)$$

with the initial conditions

$$u_D(0) = 1, \quad u_A(0) = u_k(0) = 0, \quad (13)$$

provided that the excitation is transferred to MC from the donor molecule.

Typically, biomolecules contain a huge number of structural elements, i.e. $N \gg 1$, then it is possible to use the following limit expression

$$\frac{1}{N} \sum_{k=-\pi/R}^{\pi/R} C_k \rightarrow \frac{R}{2\pi} \int_{-\pi/R}^{\pi/R} C(k) dk. \quad (14)$$

Taking this expression into account, from the system of equations (12) with boundary conditions (13) we obtain a system of integro-differential equations for the amplitudes $u_D(t)$ and $u_A(t)$:

$$\begin{aligned} \frac{du_D(t)}{dt} &= -i \left\{ \varepsilon_D u_D(t) + \int_0^t [\lambda_{11}(t-\tau) u_D(\tau) + \lambda_{12}(t-\tau) u_A(\tau)] d\tau \right\} \\ \frac{du_A(t)}{dt} &= -i \left\{ \varepsilon_A u_A(t) + \int_0^t [\lambda_{21}(t-\tau) u_D(\tau) + \lambda_{22}(t-\tau) u_A(\tau)] d\tau \right\} \end{aligned} \quad (15)$$

where

$$\begin{aligned}\lambda_{11}(t) &= |\delta_D|^2 e^{-i\Delta t} J_0(Lt), \quad \lambda_{12}(t) = i^{n_2-n_1} \delta_D \delta_A^* e^{-i\Delta t} J_{n_2-n_1}(Lt), \\ \lambda_{21}(t) &= i^{n_1-n_2} \delta_A \delta_D^* e^{-i\Delta t} J_{n_1-n_2}(Lt), \quad \lambda_{22}(t) = |\delta_A|^2 e^{-i\Delta t} J_0(Lt),\end{aligned}\quad (16)$$

$J_n(t)$ stands for the Bessel function of the first kind of the n -th order, while

$$u_k(t) = e^{-i\omega_k t} \cdot \int_0^t [V_D^*(k) u_D(\tau) + V_A^*(k) u_A(\tau)] e^{i\omega_k \tau} d\tau. \quad (17)$$

To solve such a system of equations with integrals in the form of a convolution, it is convenient to use the Laplace transform method:

$$F(p) = \mathcal{L}\{f(t)\} = \int_0^\infty e^{-pt} f(t) dt, \quad (18)$$

which is defined in the half-plane $\text{Re } p = a > s_0$, where s_0 being the growth rate of $f(t)$. As the result, the Laplace transforms of the donor and acceptor amplitudes can be presented in the form:

$$\begin{aligned}U_D(p) &= [p + i(\varepsilon_A + \Lambda_{22}(p))]/\Omega(p), \quad U_D(p) = -i\Lambda_{21}(p)/\Omega(p), \\ \Omega(p) &= [p + i(\varepsilon_D + \Lambda_{11}(p))][p + i(\varepsilon_A + \Lambda_{22}(p))] \\ &\quad + \Lambda_{12}(p)\Lambda_{21}(p),\end{aligned}\quad (19)$$

where $\Lambda_{ij}(p)$ are the corresponding Laplace transforms of $\lambda_{ij}(t)$ in Eqs. (16).

The time dependence of the amplitudes $u_D(t)$ and $u_A(t)$ is found by the inverse Laplace transform of Eqs. (19), which can be calculated using the Mellin formula

$$f(t) = \mathcal{L}^{-1}\{F(p)\} = \frac{1}{2\pi i} \cdot \lim_{b \rightarrow \infty} \int_{a-ib}^{a+ib} e^{pt} F(p) dp. \quad (20)$$

3. Phenomenon of Quantum Entanglement in Biomolecules

In the model, we consider the possibility of generating quantum entanglement as one of the most important types of quantum correlations. Quantum entanglement in biomolecules expresses the fact that the quantum state of each of its structural element cannot be described independently of the states of other structural elements. As a measure of entanglement, it is convenient to use the logarithmic negativity based on the logarithm of the trace norm of the partially transposed density matrix [5]

$$E_N(\hat{\rho}) = \log_2 \|\hat{\rho}^{PT}\| = \log_2 [1 + 2N(\hat{\rho})], \quad (21)$$

where $N(\hat{\rho}) = |\sum_i \mu_i|$ is called negativity and $\mu_i < 0$ are negative eigenvalues of $\hat{\rho}^{PT}$, which elements are defined as follows

$$\hat{\rho}_{\mu\nu}^{PT} = \hat{\rho}_{\mu\nu}. \quad (22)$$

In the case of a wave function of the form (9), the logarithmic negativity between the donor and acceptor as a function of time is given by the expression

$$\begin{aligned}E_N(t) &= \log_2 [|u_D(t)|^2 + |u_A(t)|^2 \\ &\quad + \sqrt{(1 - |u_D(t)|^2 - |u_A(t)|^2)^2 + 4|u_D(t)|^2 |u_A(t)|^2}].\end{aligned}\quad (23)$$

The emergence of quantum entanglement between the donor and acceptor in charge or energy transport processes means the formation of a quantum channel between them through which quantum information can be transmitted as well. In addition, the donor and acceptor, attached in different parts of the MC, can be considered as detectors for diagnosing quantum entanglement between the structural elements of the MC.

4. Results

As an example of MC, we consider a model of a protein-like molecule. In the case of proteins, one can associate MC excitations with peptide bond vibrations, e.g., C=O, known as Amide I. The energy of such vibrations, corresponding to the intramolecular interaction $\hbar\Delta$, is 0.21 eV, while the energy of the peptide bonds that link two consecutive amino acids into a protein chain, representing intermolecular interactions $\hbar L/2$, is estimated as 140 –

400 kJ/mol, i.e. 1.45 – 4.15 eV. Thus, in the model we assume the following relationship between the parameters: $\Delta = 0.1L$. For the model parameters of energies of the donor and acceptor molecules and their couplings with MC in sites $n_1 = 1$ and $n_2 = 5$ we adopt the following values: $\varepsilon_D = \varepsilon_A = \Delta$ and $\delta_D = \delta_A = L/4$.

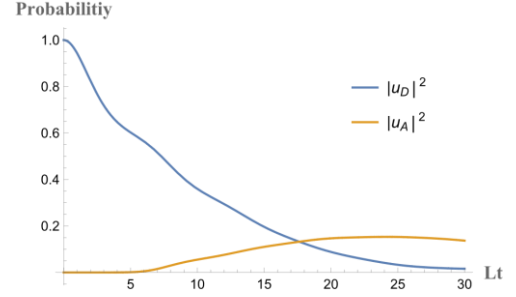


Fig. 1. Probability of finding the excitation on donor and acceptor molecules as a function of scaled time, Eqs. (19), (20).

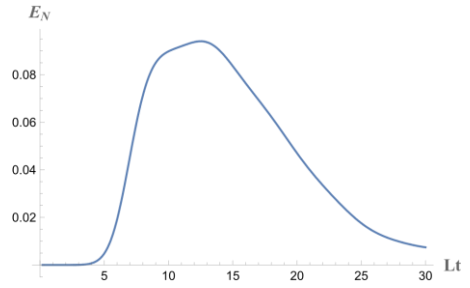


Fig. 2. Logarithmic negativity between donor and acceptor molecules as a function of scaled time, Eq. (22).

The results of the numerical calculation performed for this model with the chosen parameter values are shown in Figs. 1 and 2. Fig. 1 demonstrates the temporal migration of excitation from the donor molecule, where it was originally located, to the acceptor molecule along MC. As can be seen, despite the significant length of MC, the probability of detecting excitation on the acceptor molecule can reach tens of percent, which is due to the quantum nature of the transport process. It is important to note that during such migration, quantum entanglement arises between the donor and acceptor molecules, that indicates the formation of the quantum channel between them, which can be used to transmit quantum information, Fig. 2. The figures also show that the emergence of quantum entanglement occurs with some delay from the beginning of migration, which is related to the time required for excitation to reach the acceptor molecule in the process of its transport along MC in accordance with the evolution of the wave function (9) in time. The duration of the entanglement effect far exceeds the characteristic lifetime of excitation on the site ($\tau \sim 1/L$), which may indicate its relatively stable nature.

5. Conclusion

The report proposes a model for describing quantum correlations that can arise during the process of donor-acceptor transport in biomolecules. The emergence of non-local quantum entanglement in molecular systems is of interest from the view point of using such a quantum channel for the exchange of quantum information necessary for the stable functioning of biological objects.

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Finite Elements Modelling for Calculation of Magnetic Fields in Magnetoencephalography

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Abstract: The present study concerns the simulation, in two dimensions, by the finite element method, of the behaviour of the magnetic field created by sources of equivalent neuronal currents by considering a simplified model of a diagnostic device used in MEG (Magnetoencephalography). The simplified geometric model is composed of the head, the magnetic field sensors and the sources of equivalent currents representing the neurons. The geometric model of the head is represented by 3 layers which are brain, bone and skin. The sensors placed above the part of the skin make it possible to calculate the electric voltage induced by the magnetic field resulting from the sources of equivalent currents produced by the neurons. Neurons are represented by equidistant point current sources. The Maxwell-multi physics software has been used.

Keywords: FINITE ELEMENT METHOD, MAGNETOENCEPHALOGRAPHY, INDUCED VOLTAGE, SQUID SENSOR, HEAD AND SOURCE MODEL.

1. Introduction

The human brain is the most complex organized structure known to exist, and, for us, it is also the most important. There are at least 10¹¹ neurons in the outermost layer of the brain, the cerebral cortex. These cells are the active units in a vast signal handling network, which includes 10¹² interconnections or synapses. When information is being processed, small currents flow in the neural system and produce a weak magnetic field which can be measured noninvasively by a SQUID magnetometer, placed outside the skull, provided that thousands of nearby neurons act in concert. This method of recording, called magnetoencephalography (MEG), has already produced several pieces of new information about the functioning of the human brain. In many MEG measurements, an area in the brain that has been activated by a stimulus, such as a sound or a picture, can be located by analyzing the detected magnetic fields [1].

MEG also aids in diagnosing and delineating multiple novel findings in other neuropsychiatric disorders, including Alzheimer's disease, Parkinsonism, Traumatic brain injury, autistic disorders. If the primary source and the surrounding conductivity distribution are known, the resulting magnetic field can be calculated from Maxwell's equations. [2-3]

In the current study, we focus on the simulation 2D of the behavior of the magnetic field generated by equivalent neuronal current sources using the finite element method. It considers a simplified model of a diagnostic device used in MEG (Magnetoencephalography). The simplified geometric model comprises the "head," magnetic field sensors, and equivalent current sources representing neurons. The "head" model is represented by three layers: the brain, bone, and skin. Sensors placed above the skin layer allow for the calculation of the electrical voltage induced by the magnetic field resulting from the equivalent current sources produced by the neurons. The neurons are represented by equidistant point current sources. The study investigates the effect of the sensor position relative to the outer layer (skin) on the intensity of the calculated signal. The variation of the electrical voltage at the sensors as a function of the distance between the outer layer and the sensors is thus provided. The electrical voltage and magnetic field distribution were calculated for different situations related to the activation of a subset of neurons. The results obtained are considered consistent with those already existing in the scientific literature.

2. Geometric model of the head

Most models used today consider the head to be composed of a series of interdependent layers, each with its own physical properties, and then the model is characterized by the geometry of the interface between two continuous media [4].

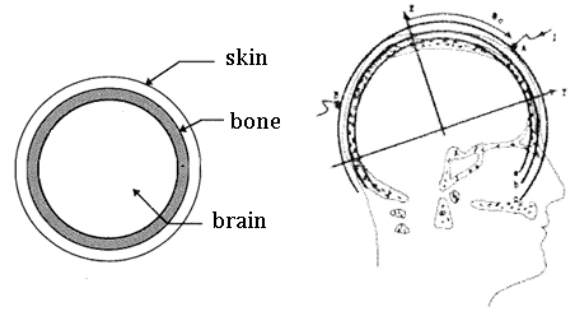


Fig. 1 Model of concentric spheres.

This model is only a very rough approximation of the head's geometry. The value of the normalized radii that we considered for our spherical model are given in Table 1.

Table 1: Normalized radii values for a three-layer model.

Medium	Scalp	Bone	Cortex
Normalized radii	1	0,92	0,87

3. Magnetostatic field computation

The modeling of the electromagnetic problems is based on the Maxwell's equations. In case of magnetostatic hypothesis we have Ampere's law, and the law of conservation of magnetic flux [5]:

$$\vec{\nabla} \wedge \vec{H} = \vec{J} \quad (1)$$

$$\vec{\nabla} \cdot \vec{B} = 0 \quad (2)$$

$\vec{H}$, $\vec{B}$ and $\vec{J}$ are the magnetic field [A/m], magnetic flux density [T] and current density [A/m²] vectors respectively.

The relation between magnetic flux density with the magnetic field which represent the medium law is given follow:

$$\vec{B} = \mu \vec{H} \quad (3)$$

μ is the magnetic permeability [H/m].

The solution of field problems that include discrete current carrying regions demands the use of the magnetic vector potential $\vec{A}$ concept.

$$\text{From (2); we deduce: } \vec{B} = \vec{\nabla} \wedge \vec{A} \quad (4)$$

4. Finite elements formulation

The behavior of the magnetic field produced by the sources of equivalent currents relative to the neurons is translated by partial

differential equations, which are obtained from Maxwell's equations (1) and (2) associated with the relations of the medium given by equation (3). In this case, the unknown variable to be considered is the magnetic vector potential $\vec{A}$.

The magnetostatic equation developed in cartesian coordinates is given by the following expression:

$$-\left(\frac{\partial}{\partial x}\left(v \frac{\partial A_z}{\partial x}\right) + \frac{\partial}{\partial y}\left(v \frac{\partial A_z}{\partial y}\right)\right) = J_{sz} \quad (5)$$

Where $v = \frac{1}{\mu}$ is the reluctivity.

The integral formula of equation (5) is given below:

$$\iint_{\Omega} \alpha_i \left(\left(\frac{\partial}{\partial x}\left(v \frac{\partial A_z}{\partial x}\right) + \frac{\partial}{\partial y}\left(v \frac{\partial A_z}{\partial y}\right) \right) + J_z \right) dx dy = 0 \quad (6)$$

Equation (6) can be rewritten in the following form:

$$\iint_{\Omega} \alpha_i \left(-\frac{\partial}{\partial x}\left(v \frac{\partial A_z}{\partial x}\right) - \frac{\partial}{\partial y}\left(v \frac{\partial A_z}{\partial y}\right) \right) dx dy = \iint_{\Omega} \alpha_i J_z dx dy \quad (7)$$

The application of Green theorem in the first term of equation (7) allows us to written:

$$\iint_{\Omega} v \left(\frac{\partial \alpha_i}{\partial x} \frac{\partial A_z}{\partial x} + \frac{\partial \alpha_i}{\partial y} \frac{\partial A_z}{\partial y} \right) dx dy - \int_{\Gamma} v \frac{\partial A_z}{\partial n} \alpha_i d\Gamma = \iint_{\Omega} \alpha_i J_z dx dy \quad (8)$$

By considering homogeneous boundary conditions, the previous relation is reduced to:

$$\iint_{\Omega} v \left(\frac{\partial \alpha_i}{\partial x} \frac{\partial A_z}{\partial x} + \frac{\partial \alpha_i}{\partial y} \frac{\partial A_z}{\partial y} \right) dx dy = \iint_{\Omega} \alpha_i J_z dx dy \quad (9)$$

$$A_z = \sum_{j=1}^n \alpha_j A_j \quad (10)$$

$A_z(x, y)$ is the unknown.

α_i is the projection function at node i.

α_j is the shape function at node j.

A_j is magnetic vector potential unknown at node j.

after introducing the magnetic vector potential discretized formula in equation (1) and with some arrangements we obtain the complex magnetostatic algebraic system to solve:

$$[M][A] = [K] \quad (11)$$

Where [M] is stiffness matrix, [K] is source vector and [A] is vector of magnetic vector potential unknowns

$$M_{ij} = \iint_{\Omega} v \left(\frac{\partial \alpha_i}{\partial x} \frac{\partial \alpha_j}{\partial x} + \frac{\partial \alpha_i}{\partial y} \frac{\partial \alpha_j}{\partial y} \right) dx dy \quad (12)$$

$$K_i = \iint_{\Omega} \alpha_i J_z dx dy \quad (13)$$

5. Induced voltage computation

The induced voltage is evaluated using Lenz's and Faraday's law, given by:

$$e = -\frac{d\Phi}{dt} \quad (14)$$

$$\Phi = \int B \cdot ds \quad (15)$$

By combining equation (14), (15) and (4), we obtain the relation which allows us to calculate the induced voltage given by:

$$V = \frac{1}{\Delta t} \int \vec{A} \cdot d\vec{l} \quad (16)$$

6. Application and results

The configuration shown in figure (2) consists of three layers representing the skin or scalp, the skull bone, and a medium for all brain tissue. The sensors are distributed over the external surface of the head.

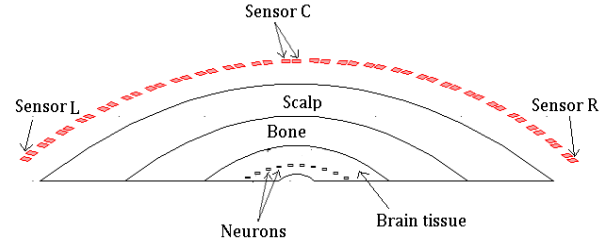


Fig. 2 Geometry of the studied problem.

The physical and geometrical proprieties for each layer are listed in Table 1.

Table 2: Geometrical and physical parameters.

Medium	Scalp	Bone	Cortex	Sensor	Neurons
Electrical conductivity [S/m]	0,33	0,00492	0,33	$5,6 \cdot 10^8$	0
Width [mm]	-	-	-	0,01	0,005
Thickness [mm]	0,1	0,092	0,087	0,01	0,005
Current density [A/m ²]	-	-	-	0	0,001

For this application, the equivalent current sources are considered constant ($J=0,001$ A/m²), and the magnetic flux density distribution is shown in Fig. 3.

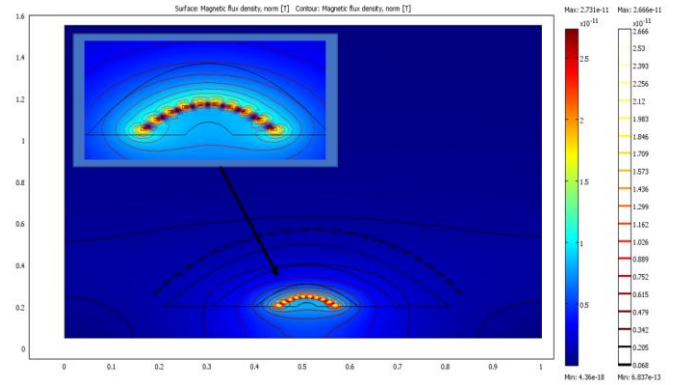


Fig. 3 Magnetic flux density distribution.

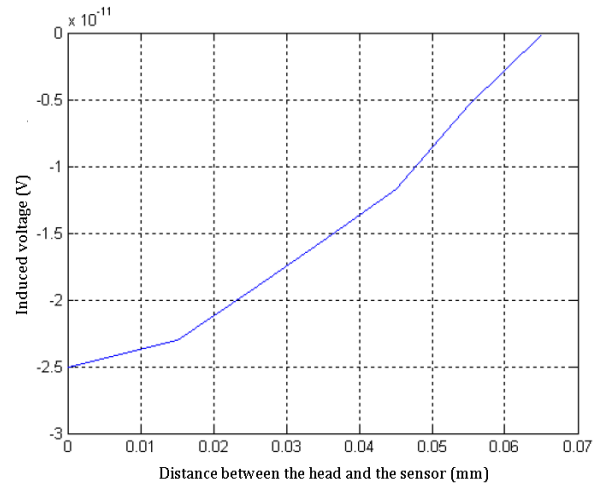


Fig. 4 Induced voltage variation as a function of distance.

The study of the effect of the position of the sensors relative to the external layer which is the skin on the intensity of the calculated signal has been highlighted, we observe a decrease in the intensity of the magnetic field (see Fig 4). The result obtained is considered to be consistent with those already existing in the scientific literature.

The magnetic flux density distribution for several values of the distance separating the sensors from the head is shown in Fig. 5.

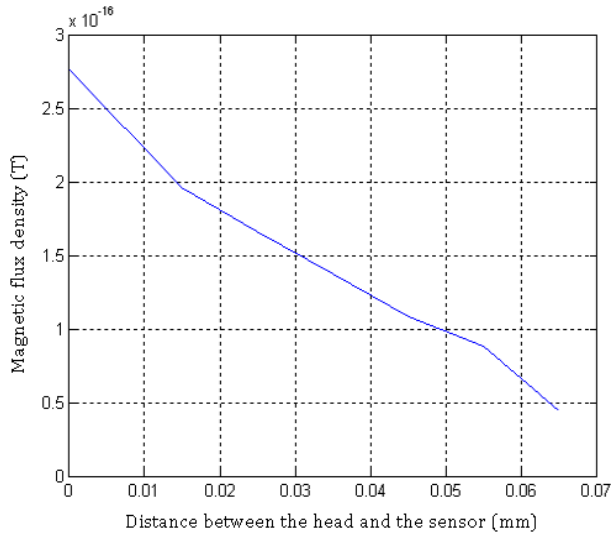


Fig. 5 Magnetic flux density variation as a function of distance.

7. Conclusion

In this work, a simplified model representing a diagnostic device used in magnetoencephalography (MEG) was analyzed using a numerical method (finite element method), and the magnetic behavior of the system was highlighted. The effect of the distance between the sensors and the outer layer of the "head" was presented, as well as the distribution of the magnetic quantity in the $[x,y]$ plane of study. The results obtained are consistent with those reported in the scientific literature.

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Mechanical Behavior of Vein under Medical Compression Stocking. Preliminary Numerical Investigations

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Abstract:

This work presents a numerical Finite Element Modeling of mechanical behavior of a human vein under influence of medical compression sock. The FE Model is developed in form of structural transient analysis by help of program product Ansys. The geometry of the vein and the muscle is assumed as an idealized, and consists of two coaxial cylinders. The stocking pressure is translated to the vein through the muscles contractions, surrounding tissues and the skin. Moreover, such a pressure and its variations, as well the position of the vein in the muscle environment, should also have influence on the functioning of venous valves and on the lymphatic system drainage. Because of preliminary character of this elaboration, these aspects are not discussed here.

The work set-up aims to establish principally how the stocking pressure loads the vein wall depending on different venous elasticity under given constant muscle elasticity.

The mechanical behavior of vein possessing elastic module $E=30\text{kPa}$ and 100kPa is considered under stocking pressure $P_{st}=25\text{mmHg}$ and 60.8mmHg and muscle tissue with elastic module $E_m=12\text{kPa}$. The displacements in the vein and muscle with corresponded distributions of stress and strain states are identified in the both two elements.

It is concluded, that these two pressures induce similar stress values in the vein walls depending on the two venous elastic modules, correspondingly. Based on that, it is suggested that a 3-Dimensional space of the geometry, pressure and the elastic modules could be existed. In such a space, optimal patient-orientated values of the pressure depending on the geometrical sizes and elasticity should be available.

Keywords: Venous ELASTICITY, Venous Surrounding tissue ELASTICITY, STRUCTURAL ANALYSIS, Finite Element Modeling

1. Introduction

In XVII century William Hardy had found unidirectional blood flow in the human body because of the presence of valves [1].

In the vein the unidirectional transport is ensured by venous valves. A human vein and valve clinically observed are given in Fig. 1. The work of venous valve is numerically modeled in [2]. Non-closure of the venous valve leads to venous reflux as seen as yellow color in Fig. 1. A basic characteristic of the venous insufficiency is the retaining of blood in the capillaries and in the surrounding tissues. Such a retaining causes increase in the capillary pressure and succeeding swelling. The systematic retaining of the blood lead to appearance of oedema [3].

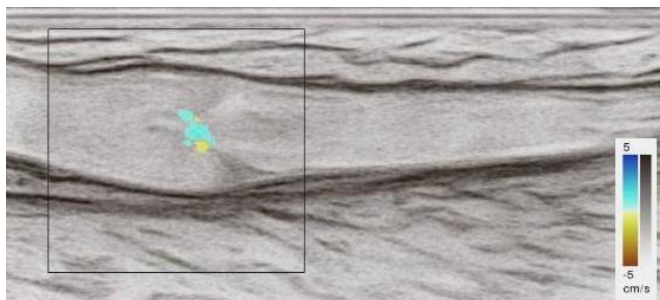


Fig. 1. Clinically observed vein and venous valve demonstrating blood reflux

Because of these circumstances the medical compressive therapy (Table 1) appears as a proper one for keeping the above pointed difference in the pressure and assures the drainage.

At this model, Fig. 2, venous valves are excluded. The pressure (Table 1) acting outside the surface of Volume 2 is transmitted by the tissues of this volume to the venous wall of Volume 1. This pressure could trans-murally lead to changes in the inside venous diameter, respectively in the venous lumen will influence the circulation and subsequent damages the venous valves.

Table 1. Ranges of Medicine Compression Stocking, [SIGVARIS]

Compr. Class for:	Compr. Mercury Column	Min Compr Pascal	Max Compr Pascal	Aver. Compr. Pascal
Prophyl axis	13 mmHg	1729		
Prophyl axis	18 mmHg	2394		
Travel	15-18 mmHg	1995	2394	2194.5
CCL1	18-21 mmHg	2394	2793	2593.5
CCL2	23-32 mmHg	3059	4256	3657.5
CCL3	34-36 mmHg	4522	6118	5320
CCL4	> 49 mmHg	> 6517		
Varix Ulcers	CCL1+(23-32)=53mmHg	7049		

The aims of this work are limited to (1) numerical developed model which should numerically describe (2) how the external surface of stocking pressure (Table 1) is transmitted from outside the skin surface through the tissue itself to the outside venous wall; (3) how the venous wall intra-murally transmit this pressure to the inside.

It is well known that, the new developed models (as well the theories!) are based on simplified idealized assumptions. Usually, that models are graphically presented, and often give adequate explanations, as well directions of future investigations. The proposed model is developed from such points of view.

2. Problem discussion

In their nature the described phenomenon present a combination of complex physico-chemical and biological live processes, and they are developed in a system "vein-environment tissues" in which deformation processes are initiated and advanced. That all is

performed with one only goal, namely – to keep the matter where they are developed alive. To achieve this goal it is extremely needed and important, that a big part of the processes to be strongly developed in acceptable limits of equilibrium, Fig. 3. To large extension these limits are determined by the range of variation of the applied external load, as well as the range of variation of the geometry and material properties of the elements in the system.

A structural analysis is performed in this work because the attention is concentrated on the deformation behavior of the two elements with different elasticity only as response of the surface stocking pressure. In fact, there are complicated fluid-structural interactions during the venous blood transport. That effects are not discussed here. The work has a preliminary character because the aims are to find venous deformations related to the different elasticity and to suggest possible negative effects on the venous wall. Enlargement and complicating of this work taking into account the above circumstances could be a subject of next works.

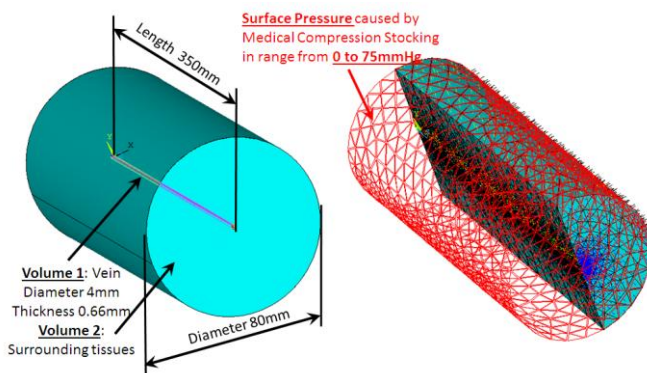


Fig. 2 Geometry of the FE model and Loads

The real structural composition of Volume 2 (surrounding/environment tissue of the vein) contains as materials besides derma, muscles, bones and lots of fine blood system and lymphatic system. The compression on the outside surface of this volume means practically compression on these structural elements numbered in itself. Under normal work conditions the peripheral capillary blood system supplies nutritive substances to the tissues in Volume 2, and the lymphatic system drains surplus amounts of lymphous fluid from the same volume.

In reality the venous structure is very complex and specific for each human individual, respectively it is very difficult to build a total numerical approximation to a given real case. Here, a vein with diameter of 4mm, thickness of 0.66mm and length 350mm is treated under surrounding tissue possessing outside diameter of 80mm and the same length of 350mm, Fig. 2. Generally, the veins are situated under intramuscular and inter-compartment conditions. At the second, the influence of the environmental elements as arteries, bones, skin, fats, fascia etc. is directly applied on the outside vein wall. These two common cases will not be separately discussed in this work. These two common cases will not be separately discussed in this work. The venous Volumes 1 and 2 are separated in 97791 and 246990 finite elements with 189247 and 342920 nodes, correspondingly. Boundary conditions of zero-displacement and symmetry are applied in the two ends of the Volumes 1 and 2. Contact conditions are applied between outside surface of Vol. 1 and inside surface of Vol. 2.

In the numerical investigations of deformation processes, the material's mechanical behavior under external loads is usually described by help of materials' models. There exist, and there are continuously developed [3] great number of materials' models of biological tissues including such ones of vascular origin. The classical linear Hook's material model is assumed in this work for both the vein and its surrounding tissue taking into account the preliminary type of this work. It determines a linear dependency between the stress state and strain state in given material, and both the states are related through Elastic module which is characteristic for each material.

In Fig. 3, experimentally obtained stress-strain diagrams (broken black step-like line) under uniaxial tension of venous sample are given. Based on these lines linear elastic (Hook's, green ellipse) and hyperelastic (5-parameter Mooney-Rivlin, thin blue line and numbers) material models are derived.

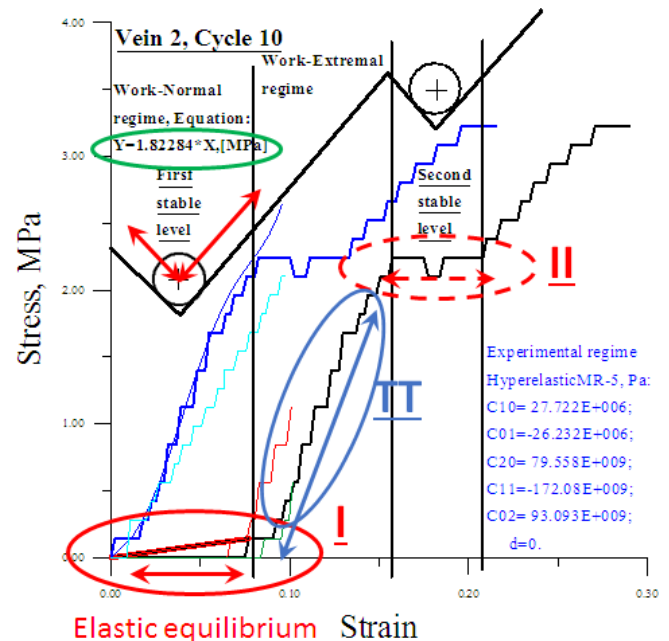


Fig. 3. Experimentally obtained stress-strain diagram by venous sample. Linear and Mooney-Rivlin elastic materials' models of vein demonstrating stable equilibrium and transitional regime of loading.

Two I and II stable equilibrium elastic regimes (red ellipses) of experimental venous behavior are seen. Above the diagram the two regimes are graphically illustrated by deviations of boll from its equilibrium state on the sloped surface. Four structural levels of deformation are established depending on corresponding regimes of increasing strain values. The first (I) equilibrium regimes is read under strain values until 0.08. After that, a transitional (TT) regime is seen up to strains 0.15 under acute increased stresses. With next increasing strains from 0.16 to 0.21, a second (II) equilibrium regime is read under relatively low increasing stresses. The rupture regime of this venous sample is established under increased strain value of 0.3.

Three levels of venous insufficiency are identified according to [4] depending on experimentally established venous elastic modules lower than 30kPa. Above 30kPa and upper 100kPa the vein is discussed as a normal. In this work the deformation behavior of vein with elastic modules of 30 and 100kPa assumed as limiting is numerically modeled under increasing compressive stocking pressure from 0 to 75mmHg (Table 1) applied on the outside surface of surrounding tissue with elastic module of 12kPa.

Strain enlargement process and form change process are simultaneously developed in Vols 1 and 2 as effect of external pressure. The stability of deformation process depends on loss of stability of one in between both the processes. The loss in strain enlargements leads to strain localizations in and ruptures. The loss of form-change leads to wrinkles and warps, compromised damaged forms and fractures.

Equilibrium equations are solved under the corresponding boundary conditions, and as result corresponding node displacements, Figs 4 and 5, with corresponding stress strain distributions, Figs 6 and 7, are obtained relating the vein deformation behavior to stocking compression Fig. 2 and Table 1, depending on the assumed elastic material models for the vein and the tissue.

3. Objective and research methodologies. Results

The numerically obtained displacements in the vein and the surrounding tissue are "conditionally" presented in macro-, mezo-

and micro-levels related to opportunity similar experimental ones to be clinically observed.

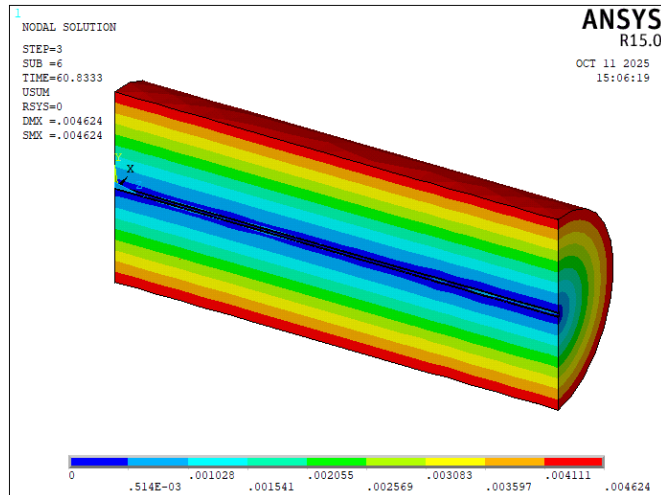


Fig. 4. Macro-level of the displacements in vein with Evein=30kPa and tissues with Emuscle=12kPa under MCS of 60mmHg.

In Fig. 4 the macro-distributions of the displacements are given across and longitudinal in the vein. Concentrically decreasing values from 4mm on the surface to 0.5-1mm in the vein and closely to vein are seen. Irregular displacements are longitudinally understandable in the vein at this observation level. With decreasing scale-observations to micro-level, three areas of displacement with equal values are seen in Fig. 5. The displacement in vein with E=100kPa have regular character under the two pressures. In the vein with E=30kPa the concentration of the displacements are clearly seen with the higher load of 60mmHg.

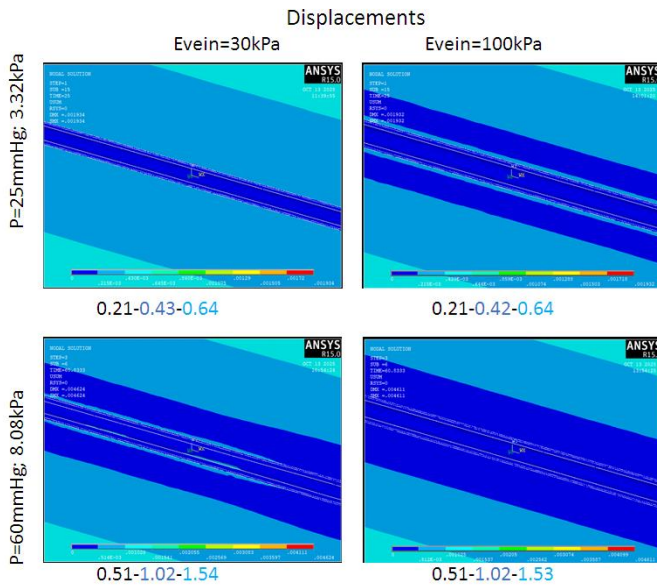


Fig. 5 Displacement, mm in meso-level in vein with Evein=30 and 100kPa and Emuscle 12=kPa under P=25 and 60mmHg.

It should be emphasized, the subject of this elaboration is concentrated on the numerically modeled deformation behavior of idealized forms of the two volumes determined by their mechanical properties. The corresponded to Fig. 5 strain- and stress-distributions are presented in Figs 6 and 7. Twice-thrice increased venous strain are seen with Ev=30kPa while the stress differences in are of one time and half. Related to strain-values in the I-equilibrium state in Fig. 3, the values higher of 0.12 for Ev=30kPa under 25mmHg and for Ev=100kPa under 60mmHg suggest

transition to the TT-stage *i.e.* start of new structural level of deformation. Strain- and stress-distributions in the surrounding tissues have close to similar characters.

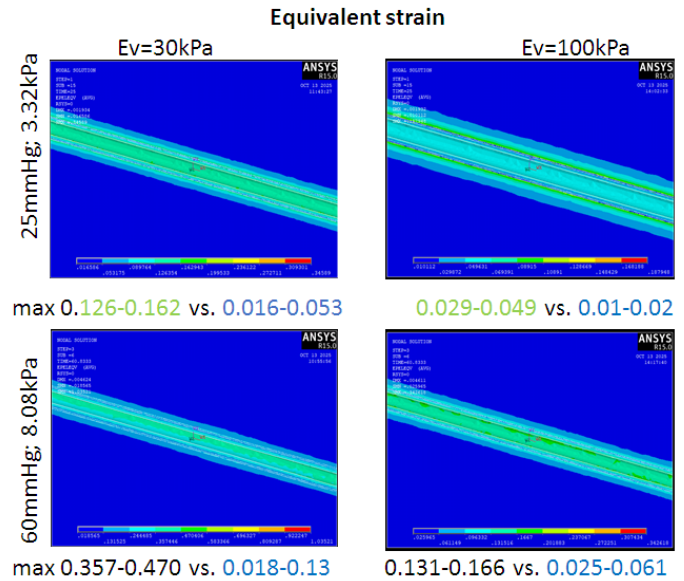


Fig. 6. Strain-distribution in meso-level in vein/tissue with Evein=30 and 100kPa and Emuscle 12=kPa under P=25 and 60mmHg.

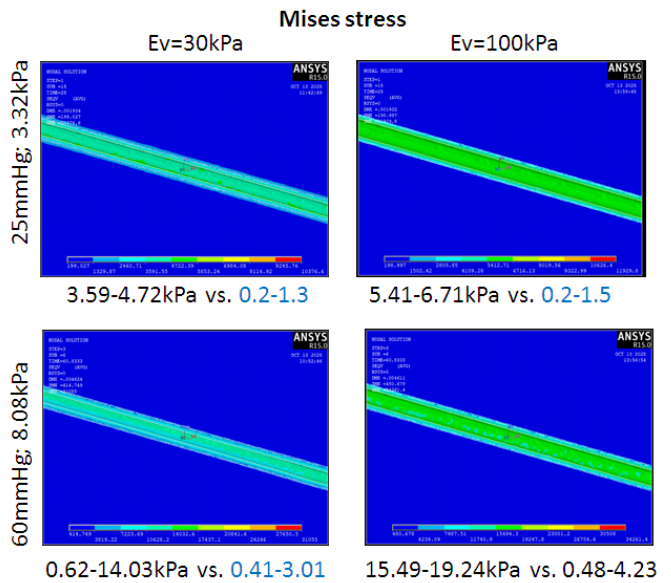


Fig. 7. Mises stress distribution in meso-level in vein/tissue with Evein=30 and 100kPa and Emuscle 12=kPa under P=25 and 60mmHg.

Next decreasing in “scale-level” numerical observation to micro-level and concentration of the attention on the vein reveal displacements and stress-strain distributions in longitudinal and trans-mural venous directions, Figs 8, 9, 10.

In Fig. 8 at P=25mmHg twice higher displacement’s values for Ev=30mmHg are seen compared to Ev=100kPa. However, in Fig. 8 the loss of stability in the circular venous form is clearly seen with Evein=30kPa under P=60mmHg. The vein with Ev=100kPa obtains more elliptical form at 70mmHg. Here, it must be strongly pointed that this surface stocking pressure is over-pressure according to Table 1, but we are here numerically looking for the limiting loading regimes depending on the venous elasticity. Such loading regimes could be related to different deformation behavior specific for given elastin-collagen contents.

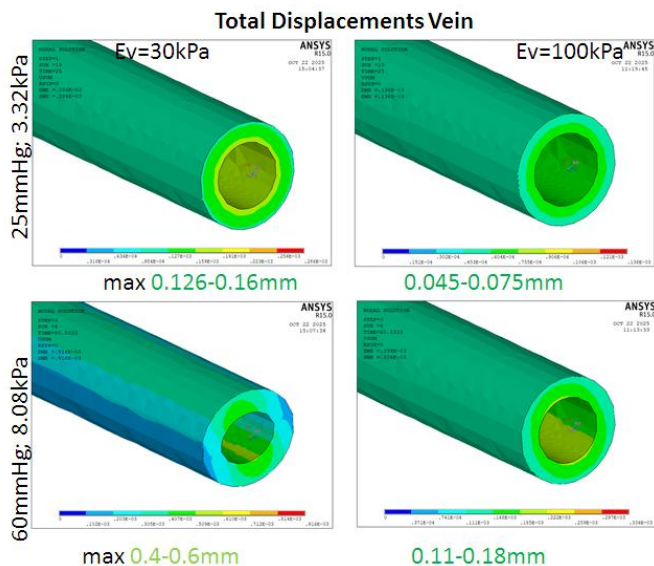


Fig. 8. Displacement in micro-level in vein with $E_{\text{vein}}=30$ and 100kPa and $E_{\text{muscle}}=12\text{kPa}$ under $P=25$ and 60mmHg .

Next, the attention on the strain values of vein with $E_{\text{vein}}=30\text{kPa}$ (Fig. 9) establish that the values of $0.031-0.066$ at 25mmHg are in the ranges of the I-rst equilibrium Work-Normal regime seen in Fig. 3, and upper value goes closely to the limit of 0.08 . Surface $P=60\text{kPa}$ leads to strain values $0.018-0.244$, where the second values indicates structural transformation in the venous wall. The surface stress values observed in Fig. 9 are approximate to the values of 3.32 and 8.08kPa (25 and 60mmHg) applied to the surface of the venous surrounding tissue

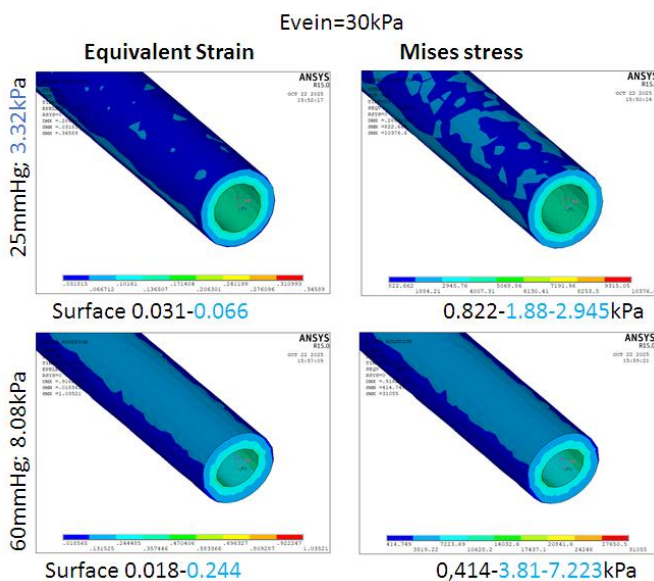


Fig. 9. Strain and stress distributions at micro-level in vein with $E_{\text{vein}}=30\text{kPa}$ and $E_{\text{muscle}}=12\text{kPa}$ under $P=25$ and 60mmHg .

Analyses of Fig. 10, as well Fig. 8, reveal a stably deformed cylindrical form of the vein with $E_{\text{vein}}=100\text{kPa}$. Looking at the strain values from $0.022-0.034$ to $0.061-0.096$ for $P=25$ and 60mmHg correspondingly, it could be concluded that the vein works under equilibrium conditions of the Ist level, Fig. 3. The venous stress values are in commensurable ranges to the surface pressure of $P=25$ and 60mmHg . They show that the surface stocking compression is transmitted by the venous surrounding tissue possessing $E_{\text{muscle}}=12\text{kPa}$ to the outside venous wall with similar values. Questions could be here imposed about these stress values, could they cause structural (elastin-collagen, including fibre tearing) transformations in the vein with $E=30\text{kPa}$ and do not cause in this

one with $E_{\text{vein}}=100\text{kPa}$. That is out of the subject of this work because of its initial work stage.

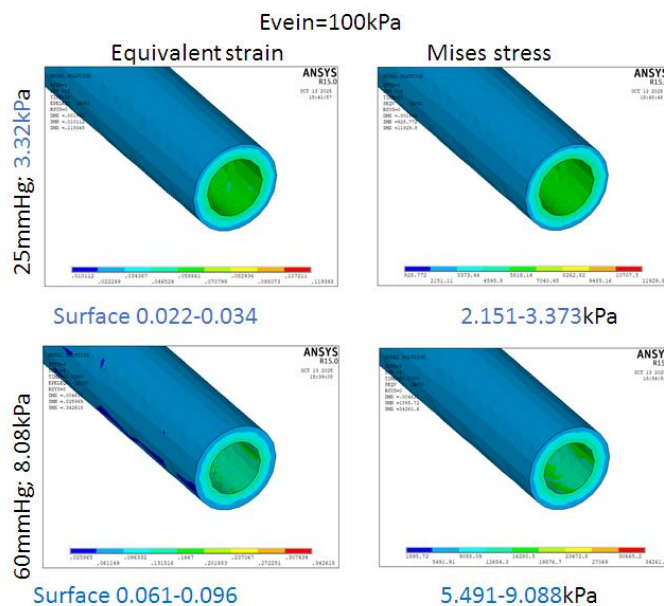


Fig. 10. Strain and stress distribution at micro-level in vein with $E_{\text{vein}}=100\text{kPa}$ and $E_{\text{muscle}}=12\text{kPa}$ under $P=25$ and 60mmHg .

4. Conclusions

A 3-D numerical simulation of mechanical behavior of vein under medicine compression stocking is developed by help of FE Modeling and Ansys program product, Fig. 2. The vein is modeled as tube with diameter 4mm , thickness 0.66mm , length 350mm and having elastic (Young) modules $E_{\text{vein}}=30\text{kPa}$ and 100kPa . The surrounding tissue of the vein has diameter 80mm , the same length of 350mm and elastic module $E_{\text{muscle}}=12\text{kPa}$. Linear elastic (Hook) materials' models are assumed, as in elastic equilibrium loading stage, Fig. 3. The surrounding-tissue surface is compressed step-by-step in range from 0 to 75mmHg , Table 1. Three levels of distributions of the displacements, strain and stress in the vein are presented under pressure $P=25$ and 60mmHg in Figs 4-11. It is established that the strains in vein with $E_{\text{vein}}=100\text{kPa}$ have values below 0.08 , as these ones characteristic for the normal elastic equilibrium loading stage given Fig. 3. With $E_{\text{vein}}=30\text{kPa}$ at pressure of $P=25\text{mmHg}$ the strains are lower than the equilibrium of 0.08 , but with increasing $P=60\text{mmHg}$ elliptical loss of stability in the venous form-change process is established at thrice higher strain 0.244 than the equilibrium limiting one 0.08 . It is established for the two venous elasticities, that all surface pressures P from 0 to 75mmHg are transmitted in similar stress values on the outside venous wall, Figs 9-10 approximately of 3.32 and 8.08kPa for cases of $P=25$ and 60mmHg . Finally, we conclude 3-D space of the geometry, pressures and elastic modules could be existed. In such a space, optimal patiently-orientated values of the stocking pressure should be available depending on the geometry and elasticity.

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Particle-in-cell modeling of non-radiating states of laser-plasma

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Abstract: In this work we study numerically, by means of Particle-in-Cell simulations, the formation of non-radiating configurations in a plasma, arising from the ionization of atomic gases by intense laser pulse. Our simulation show that, after the release of a short terahertz pulse, a nearly non-radiating field and current configuration is formed, even though the charge and current distributions of plasma remain essentially time-dependent. In a plasma target emitting terahertz waves, such a non-radiating state is formed under the action of radiation. Our calculations suggest that formation of a non-radiating configuration occurs in a self-consistent way and can therefore affect the duration of the emitted terahertz pulse.

KEYWORDS: PARTICLE-IN-CELL SIMULATIONS, TERAHERTZ RADIATION

1. Introduction

The generation of time-dependent non-radiative currents in a rarefied plasma is a rather common phenomenon. Current oscillations at a frequency at which the plasma permittivity is zero can be mentioned as a simplest example. Another, more complex example consists in the generation in an inhomogeneous plasma of a current density distribution with a vanishing dipole moment. Strictly speaking, such a configuration can not be called completely non-radiative, but since the radiation occurs because of the higher-order moments, it has a very high frequency, which is much bigger than the plasma frequency. Finally, these could be trivial configurations with an anomalously small dipole moment or cases where the propagation of the wave with a given frequency is prohibited by the dispersion relation.

In this paper we present a tool for a numerical study of time-dependent current configurations with a non vanishing dipole moment that do not emit radiation because of a complete or nearly complete destructive interference in the far-field zone. Such states – the so-called anapole states – have long been known to exist theoretically [1,2] and have been studied by several prominent scientists [3,4], including Ehrenfest, Zeldovich, and Ginzburg, but their practical realization have been realized only recently in metamaterials. For example, a review [5] discusses a small emitter (with a size on the order of a wavelength), where suppression of radiation can not be attributed to the restrictions given by the dispersion relation. In this case, the suppression occurs because the currents and charges in the emitter oscillate in a very specific way. Our calculations show that in a plasma target emitting terahertz (THz) waves, a non-radiating state may be formed under the back reaction of the THz radiation. In particular, when a THz wave is emitted from a small plasma target (with a size of the order of the wavelength of the THz wave), the back reaction of the radiation on the motion of the charged particles leads to the rapid formation of a plasma configuration that no longer emits radiation. At the same time, it continues to perform rather complex oscillations. Since in this case the formation of a non-radiating configuration occurs in a self-consistent way, it can therefore affect the duration of the THz pulse, making it very short. The structure of the paper is following. First we formulate the problem statement and present the main numerical algorithms we use. Then we discuss our numerical results and finally, report the conclusion.

2. Numerical model and Setup

The initial setup is schematically shown in Figure 1. The rectangular domain $L_{\text{domain}} \times \Delta_{\text{domain}}$ is partially occupied by a neutral gas. The laser pulse enters the domain from the left. The laser pulse is characterized by the intensity I_0 , duration τ_0 , focal spot-size r_0 , polarization (linear or circular) and spectrum (mono- or bichromatic). The gas cell - by the initial concentration n_0 , size of the cell $L_{\text{cell}} \times \Delta_{\text{cell}}$ and gas type. We assume, that the plasma, formed by the ionization, can be considered as collisionless.

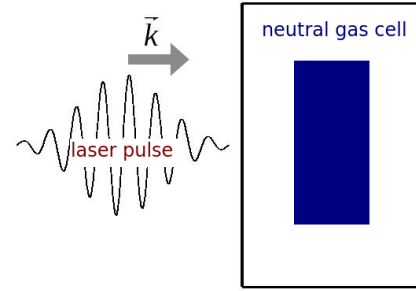


Figure 1. Initial setup: The rectangular domain is partially occupied by a neutral gas. The laser pulse enters the domain from the left and propagates to the right.

A self-consistent model to study the behavior of fully or partially ionized gases in the field of an intense laser pulse consists of Vlasov kinetic equations for the distribution functions of plasma ions and electrons and Maxwell's equations for the electromagnetic fields E, B [6].

We measure the mass and charge of the ions in the electron mass m_e and the elementary charge e , normalize the velocities to the speed of light c , use the values of the main wavelength λ_0 of the laser pulse as the length unit and the amplitude of the dimensionless vector potential $a_0 = eE_0\lambda_0/(2\pi m_e c^2)$ – as the unit for the electromagnetic field amplitude. Note that for a linearly polarized electromagnetic pulse with wavelength $\lambda_0 = 800\text{nm}$ the value $a_0 = 1$ of the normalized vector-potential corresponds to the intensity of $I_0 = 2.1 \cdot 10^{18} \text{ W/cm}^2$.

We solve the Vlasov equations using Particle-in-Cell (PIC) method [7-9] and obtain the solutions of the Maxwell equations using a finite-difference time domain (FDTD) scheme [10,11].

To solve the equations of motion for the charged particles the Boris scheme [12] is used. It is of the second order in time $O(\Delta_t^2)$, time reversible and unconditionally stable [13]. Formally, the scheme is implicit, but its implementation can be done in an explicit way. In [14] it has been proven that the long-term accuracy of the Boris algorithm is ensured because it preserves the phase space volume. In Cartesian geometry the solution of Maxwell's equations is performed on a uniform rectangular grid $x_i = i \cdot \Delta_x, y_k = k \cdot \Delta_y$, with $\Delta_{x,y}$ being the grid spacings. The values of the components of the electric and magnetic fields are defined on the staggered grids and are shifted relative to each other by a half step size in time. Since the conventional FDTD scheme [10,11] uses central differences to approximate the derivatives of the fields, it has a second order of approximation over all grid steps $O(\Delta_t^2, \Delta_x^2, \Delta_y^2)$ with Δ_t being the time step. The scheme is explicit and conditionally stable if $c\Delta_t(\frac{1}{\Delta_x} + \frac{1}{\Delta_y}) \leq 1$.

The FDTD scheme ensures an automatic fulfillment of discretized Gauss's law for the magnetic field $\nabla \cdot \vec{B} = 0$ at any time step, provided it is fulfilled at $t=0$. To guarantee an automatic fulfillment of the discrete analog of Gauss's

law for the electric field $\nabla \cdot \vec{E} = 4\pi e(Zn_i - n_e)$, where n_e is the electron concentration and n_i and Z are the ion concentration and ion charge, we use an algorithm of reconstruction of the current density first proposed in [15] and later generalized in [16]. Ionization of the gas cell by the electric field is taken into account using formulas for the tunnel ionization probability $w(E)$. These use the instantaneous value of the electric field strength [17,18], in contrast to the widely used ADK [19] formula, in which the electric field is averaged over the period. Numerically we proceed as follows. At $t=0$ the computational domain contains a neutral gas, which is modeled by identical particles having a distribution by coordinates according to the initial gas concentration $n_0(x, y)$. At each point of the domain (x_j, y_j) , occupied by a neutral atom or an ion in a low charge state the ionization probability $p = 1 - e^{-w(E)\Delta t}$ is calculated. The refection method [20] is used to decide whether the ionization event takes place or not. If an ionization event takes place, the charge state of the parent atom/ion is increased by one and an immobile "new" electron is born at (x_j, y_j) . At the next time step positions and velocities of the "new" electrons are updated and their contributions to the charge and current density are calculated. Since the intensity of laser radiation is not very high, ionization can lead to significant losses of pulse energy. To take into account the depletion of the laser pulse due to ionization losses we follow [21,22] and introduce an "ionization" current $\vec{j}_{ion}$, whose direction coincides with the direction of the electric field $\vec{E}(x_j, y_j)$ at the position (x_j, y_j) of the "parent" ion, and whose density, is such that $(\vec{j}_{ion} \cdot \vec{E}(x_j, y_j)) = W_E$, where W_E is the work of the electric field spent on ionization during the time step Δt . The energy conservation in every numerical cell is controlled: if the remaining electric field energy is not sufficient for further ionization, then no further ionization occurs.

3. Simulation results

Numerical simulations discussed below have been performed at the Joint Supercomputer Center of the Russian Academy of Sciences and at the Siberian Supercomputer Center of the Siberian Branch of the Russian Academy of Sciences. In order to efficiently use the resources provided by these Centers the numerical code has been parallelized. The details of the parallelization strategy can be found in e.g. [23]. Data exchange between processor elements is handled by means of MPI routines, FORTRAN has been chosen as the basic programming language. We performed series of simulations in a wide range of parameters, which are summarized in a Table 1 and Table 2 below. In all the simulations the laser pulse was bichromatic with a wavelength of the second harmonic $\lambda_1 = \lambda_0/2$. The amplitude of the electric field of the second harmonic was $a_1 = 0.2a_0$.

a_0	polarization	λ_0, nm	r_0/λ_0	$\tau_0 c/\lambda_0$
0.02 - 0.05	CP(LP)-LP(CP)	800 - 2000	5-50	10 - 100

Table 1: Basic parameters of the laser pulse used in simulations. Abbreviation CP/LP denotes circular/linear polarization of the laser pulse.

$n_0, 10^{18} cm^{-3}$	Δ_{cell}/λ_0	L_{cell}/λ_0	L_{domain}/λ_0	$\Delta_{domain}/\lambda_0$
1 - 20	4 - 50	5 - 200	100 - 250	100 - 250

Table 2: Basic parameters of the argon gas cell used in simulations. In Figures 2 and 3, we plot, exemplarily, the distribution of the period-averaged electric field (E_y component in Fig. 2 and E_z component in Fig. 3) for the simulation of the interaction of a circularly polarized bichromatic laser pulse with $\lambda_0 = 2\mu m, a_0 = 0.05$ with small argon cell of $\Delta_{cell} = L_{cell} = 5\lambda_0$ of the

initial concentration of $n_0 = 9 \times 10^{17} cm^{-3}$. The y- component of the electric field is show for $t = 100\lambda_0/c = 667 fs$ and the z-component of the electric field is shown at three subsequent time moments, $t = 30\lambda_0/c, 70\lambda_0/c$ and $100\lambda_0/c$. The generation and propagation of a short terahertz pulse is clearly visible.

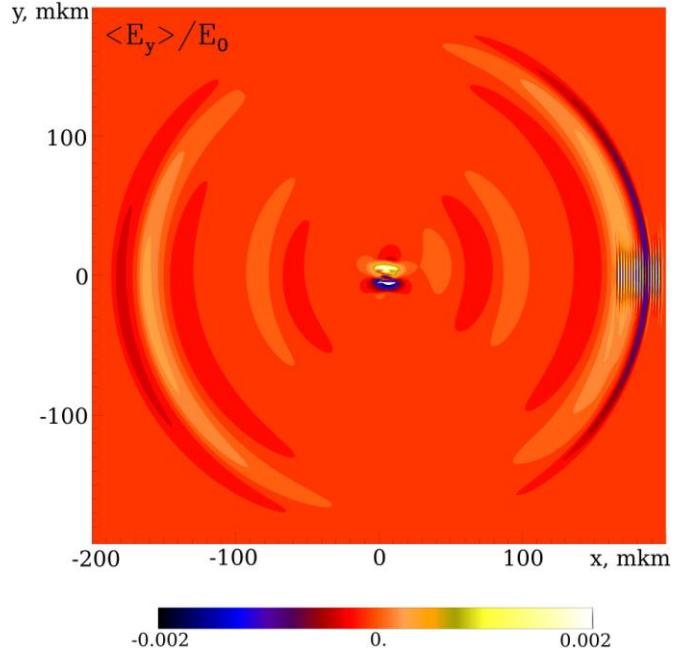


Figure 2. The distribution of the period averaged y-component of the electric field at $t = 100\lambda_0/c = 667 fs$.

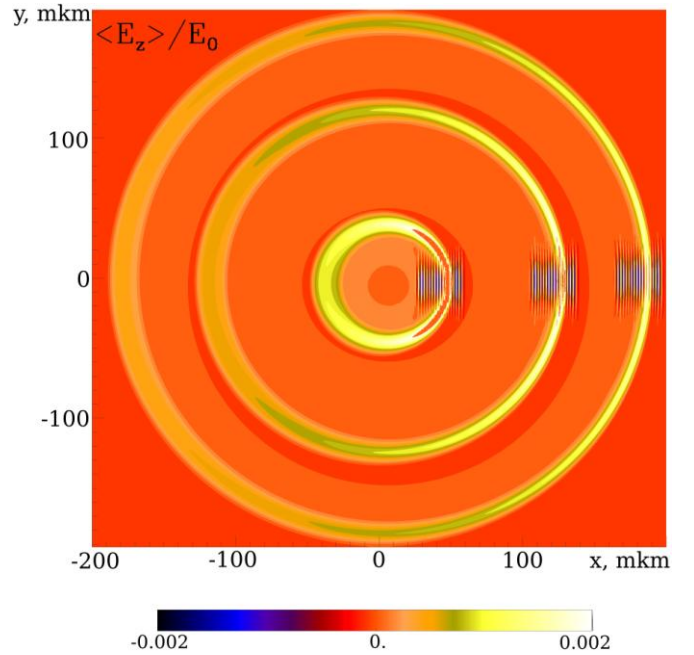
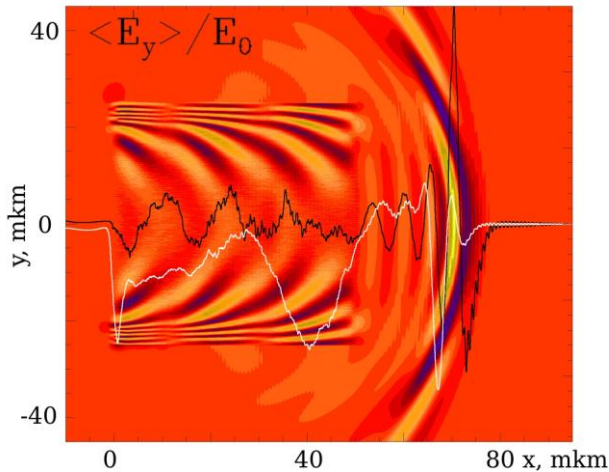


Figure 3. The distribution of the period averaged z-component of the electric field at $t = 30, 70, 100\lambda_0/c$, corresponding to 200, 467 and 667 fs.

An example of a non-radiating configuration is plotted in Figure 4. The distribution of the y-component of the electric field is shown for $t = 120\lambda_0/c = 320 fs$. Here the circularly polarized bichromatic laser pulse with $\lambda_0 = 0.8\mu m, a_0 = 0.05$ interacted with larger argon cell of $\Delta_{cell} = L_{cell} = 62.5\lambda_0$ of the initial concentration of $n_0 = 1.1 \times 10^{19} cm^{-3}$. After a release of a short terahertz pulse, this configuration doesn't emit radiation anymore, although the

distribution of the fields and currents remains essentially time-dependent.



4. Conclusion

In this paper a numerical tool to study dynamical configurations of plasma created through the ionization of an initially neutral gas cell by an intense laser pulse has been presented. The mathematical model consists of Vlasov equations for the distribution functions of the plasma species and Maxwell equations for the electromagnetic field. To solve the Vlasov equations the widely used PIC method has been applied. To self-consistently update the electromagnetic fields the FDTD method has been used. Series of simulations within the wide range of laser pulse and gas cell parameters has been performed to examine the formation of non-radiating configurations in a plasma arising from the ionization of atomic gases by an intense bichromatic laser pulse. The results of the simulations have confirmed that in the interaction of a relatively long but not monochromatic laser pulse with an initially neutral gas cell an asymmetric photoelectron momentum distribution is formed. The resulting strong, time-dependent photoelectron current leads to the emission of a short electromagnetic pulse in the THz domain. After the release of a short THz pulse, a nearly non-radiating plasma configuration is formed, even though the charge and current distributions remain essentially time-dependent. Our calculations suggest that the formation of a non-radiating configuration occurs in a self-consistent way and can therefore affect the duration of the THz pulse, making it potentially very short.

5. Funding

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Heuristic optimization of moving-average trading rules on stock data

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Abstract: This paper investigates the optimization of a Moving-Average (MA) crossover trading strategy using derivative-free methods. The strategy, defined on daily prices of the S&P 500, Apple (AAPL), and Alphabet (GOOGL) (1995–2024), is characterized by two integer parameters: short-term and long-term window lengths. We treat the in-sample annualized Sharpe ratio as a black-box objective function. We propose a multi-start coordinate pattern search algorithm that iteratively probes neighboring parameters and adaptively shrinks step sizes. Results from 1000 Monte Carlo runs per asset demonstrate that the method reliably converges to near-optimal solutions comparable to expensive brute-force grid searches. The optimizer identifies distinct optimal regimes: medium-term windows for GOOGL, a fixed long-term trend (approx. 220 days) for the S&P 500, and a specific fast-slow combination (2 and 240 days) for AAPL.

KEYWORDS: HEURISTIC OPTIMIZATION, MOVING-AVERAGE CROSSOVER STRATEGY, SHARPE RATIO, MONTE CARLO

1. Introduction

Moving-average crossover rules are foundational technical trading strategies. They generate signals by comparing a short-term moving average of price to a longer-term average, exploiting momentum. While simple, the mapping from the window parameters to risk-adjusted performance (Sharpe ratio) is non-linear, non-smooth, and non-convex.

From an optimization perspective, this presents a classic black-box problem. The objective function is discrete (integer parameters) and expensive to evaluate (requiring full historical backtests), rendering gradient-based methods inapplicable.

We formulate the parameter tuning as a derivative-free optimization task. We employ a Coordinate Pattern Search, a direct search method that navigates the parameter space using local exploration and step-size reduction. To address the multi-modal nature of the objective landscape, we utilize a Multi-Start framework. We validate the method against brute-force "Sharpe maps" (dense grid evaluations) for three distinct assets, S&P 500 (market index), AAPL, and GOOGL (tech large-caps), demonstrating the algorithm's robustness and efficiency.

2. Problem Formulation

2.1 Data and Strategy

We utilize daily adjusted closing prices (P_t) from Yahoo Finance for the S&P 500, AAPL, and GOOGL, covering Jan 1, 1995 (or the first available date), to Dec 31, 2024. Daily simple returns are defined as:

$$R_t = \frac{P_t - P_{t-1}}{P_{t-1}}$$

The strategy relies on two integer parameters, n_{short} and n_{long} , bounded such that $2 \leq n_{short} < n_{long} \leq 500$. The moving averages (MA) at time t are:

$$MA_t^k = \frac{1}{n_k} \sum_{i=0}^{n_k-1} P_{t-i}, \quad k \in \{short, long\}$$

The trading signal generates a long position when the short MA exceeds the long MA:

$$Signal_t = \begin{cases} 1, & \text{if } MA_t^{short} > MA_t^{long} \\ 0, & \text{otherwise} \end{cases}$$

To prevent look-ahead bias, the return at t is determined by the signal at $t - 1$:

$$r_t^{strat} = Signal_{t-1} \cdot R_t$$

2.2 Optimization Objective

The objective is to maximize the annualized Sharpe ratio. Let μ_{strat} and σ_{strat} be the sample mean and standard deviation of daily strategy returns. The objective function S is:

$$S(n_{short}, n_{long}) = \frac{\mu_{strat}}{\sigma_{strat}} \sqrt{252}$$

The optimization problem is defined as:

$$\max_{n_{short}, n_{long}} S(n_{short}, n_{long}) \quad \text{s.t.} \quad 2 \leq n_{short} < n_{long} \leq 500$$

3. Methodology

3.1 Benchmark: Brute-Force Sharpe Maps

To establish a ground truth, we compute the Sharpe ratio on a dense grid for all valid pairs (n_{short}, n_{long}) . This requires approximately 125,000 evaluations per asset. These "Sharpe Maps" (visualized in Figure 1, 2 and 3) reveal the non-convex landscape, characterized by ridges and multiple local maxima rather than a single smooth peak.

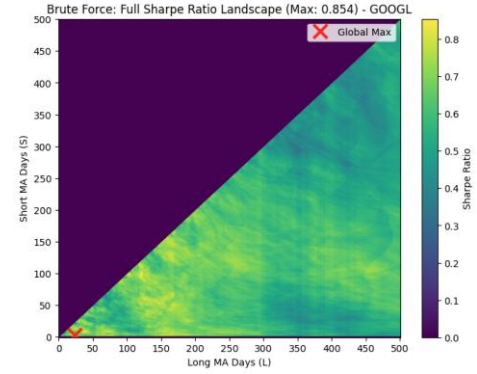


Figure 1. Sharp Heat Maps for GOOGL

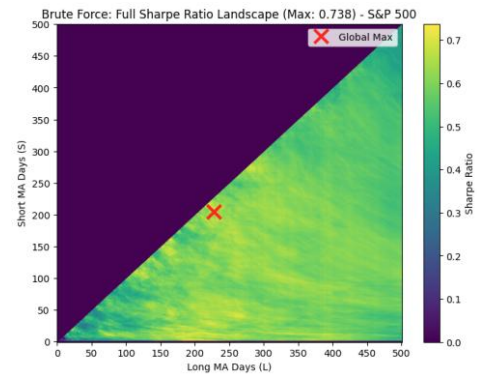


Figure 2 Sharp Heat Maps for S&P 500

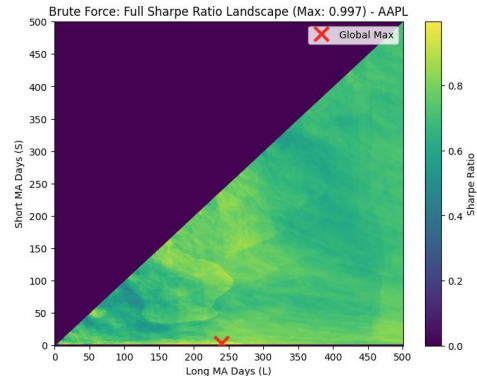


Figure 3 Sharp Heat Maps for AAPL

3.2 Algorithm: Multi-Start Coordinate Pattern Search

We employ a derivative-free pattern search that explores the integer lattice.

Single-Start Procedure:

1. **Initialization:** Start at (s_0, l_0) with initial step sizes $h_s = h_l = 80$.
2. **Poll:** Evaluate the objective at feasible neighbors: $(s \pm h_s, l)$ and $(s, l \pm h_l)$.
3. **Update:**
 - If a neighbor improves the Sharpe ratio, move to that neighbor; keep step sizes constant.
 - If no improvement is found, shrink step sizes: $h \leftarrow \max(1, \lfloor h/2 \rfloor)$.
4. **Termination:** Stop when $h_s = h_l = 1$ and no immediate neighbor improves the solution.

Multi-Start Strategy: Since pattern search can get trapped in local optima, we execute the algorithm from 10 random starting points per run. The best result among these starts is recorded as the solution for that run.

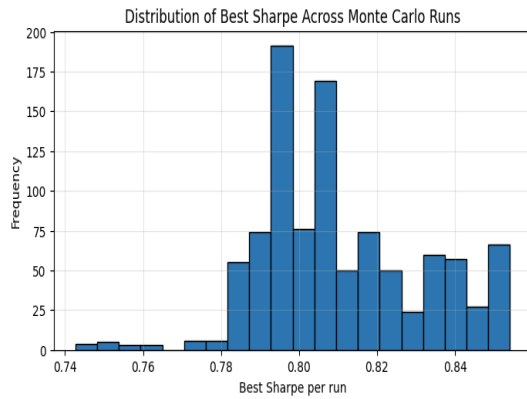


Figure 4 Distribution of Best Annualized Sharpe Ratio Across Monte Carlo Runs- for GOOGL

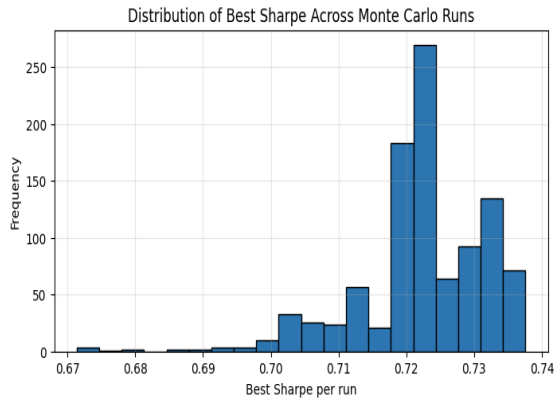


Figure 5 Distribution of Best Annualized Sharpe Ratio Across Monte Carlo Runs- for S&P 500

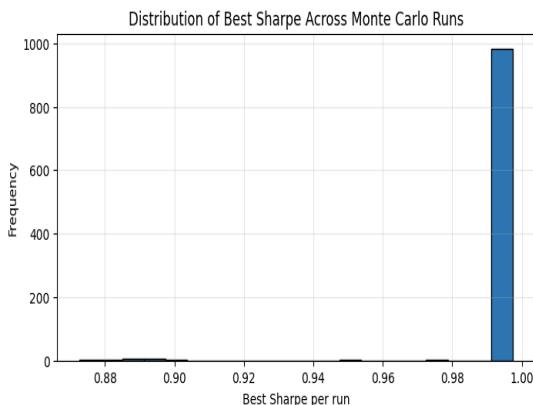


Figure 6 Distribution of Best Annualized Sharpe Ratio Across Monte Carlo Runs- for AAPL

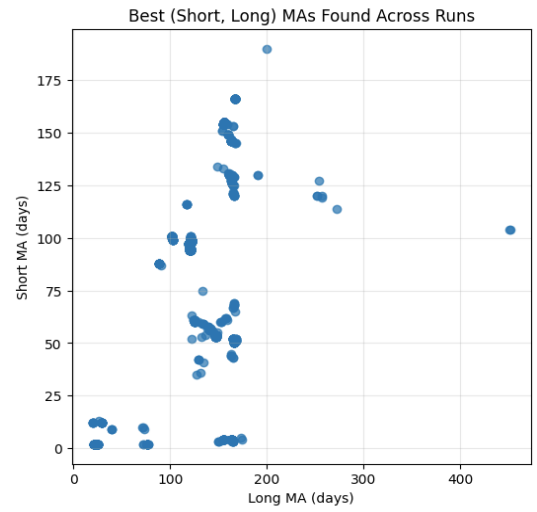


Figure 7 Parameter convergence of Best MA pairs for Across Monte Carlo Runs- GOOGL

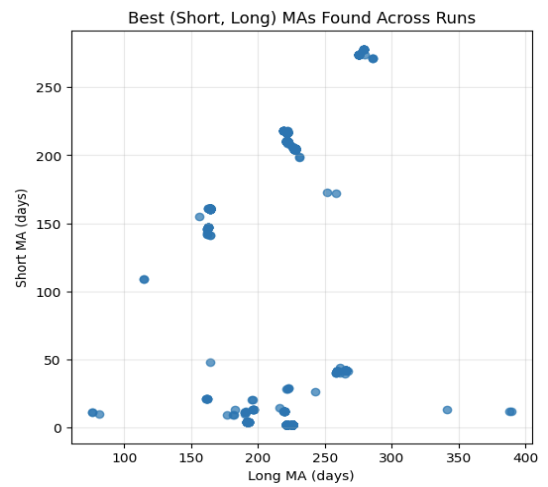


Figure 8 Parameter convergence of Best MA pairs for Across Monte Carlo Runs- S&P 500

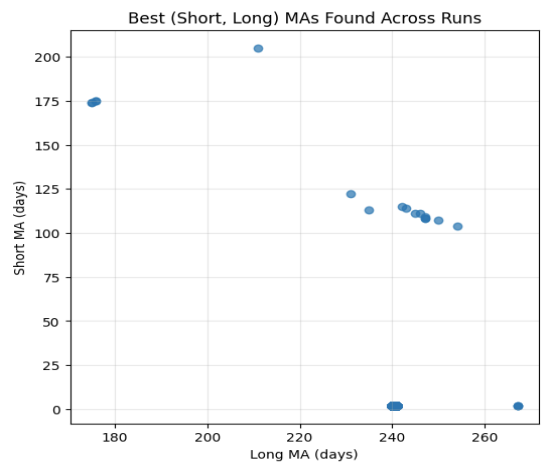


Figure 9 Parameter convergence of Best MA pairs for Across Monte Carlo Runs- AAPL

4. Empirical Results

We performed a Monte Carlo analysis consisting of 1000 independent runs per asset to assess convergence stability. Table 1 summarizes the distribution of the optimal parameters found across these runs.

Table 1: Summary of Optimization Results (1000 Monte Carlo Runs) - Mean and Standard Deviation of the best parameters found by the optimizer.

Asset	Mean Best Sharpe	Max Found Sharpe
GOOGL	0.811 ± 0.021	0.854
S&P 500	0.722 ± 0.010	0.738
AAPL	0.995 ± 0.013	0.997

4.1 Convergence Analysis

Alphabet (GOOGL): The optimizer achieves a mean Sharpe ratio of 0.811 with moderate variance (± 0.021). Analysis of the underlying parameters reveals a broad solution space; the algorithm converges to various "medium-term" window combinations that yield similar performance. This indicates a relatively flat objective surface for GOOGL, where distinct local optima offer comparable risk-adjusted returns.

S&P 500: While the Sharpe ratios are highly stable (0.722 ± 0.010), the parameter convergence highlights a distinct structural feature. The optimizer consistently pins the long window to approximately 220 days, while the short window varies significantly (spanning 2 to 200 days) across runs. This implies the existence of a "ridge" in the landscape: as long as the long-term trend is defined by a ~220-day filter, the specific choice of the short-term window has a marginal impact on the Sharpe ratio.

Apple (AAPL): AAPL exhibits the most robust convergence in both performance and parameter selection, achieving a mean Sharpe ratio of 0.995. Unlike the other assets, the optimizer almost exclusively locates a specific global maximum at the boundary: a fast short MA (≈ 2 days) paired with a long MA of roughly 240 days. The extremely low standard deviation in the Sharpe ratio (0.013) confirms that the Multi-Start Pattern Search consistently identifies this dominant peak.

5. Conclusion

This study demonstrates that multi-start coordinate pattern search is a highly effective method for optimizing technical trading rules. Despite the non-convex and non-smooth nature of the Sharpe ratio landscape, the algorithm successfully identifies robust high-performance regions.

The empirical results highlight asset-specific dynamics: AAPL benefits from reacting to long-term trends with immediate execution (2/240 crossover), while the S&P 500 allows for more flexibility in the short-term signal provided the long-term filter is set to roughly one trading year (~220 days). By treating the strategy as a black box, this derivative-free approach avoids the pitfalls of gradient-based methods and offers a computationally efficient alternative to brute-force grid searches.

6. Acknowledgement

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Topology as a lens for semantic organization in transformer embeddings

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Abstract: This paper examines the geometric structure of sentence embeddings through the lens of persistent homology. The goal is to determine whether semantic similarity produces distinctive topological patterns in a controlled embedding environment. To isolate semantic effects, a single sentence template was combined with different target words, forming two point clouds in a transformer embedding space: one derived from semantically similar words and one from dissimilar words. A Vietoris–Rips filtration was applied to both clouds, and the resulting persistence diagrams were summarized by average lifetime, entropy of birth–death intervals, and the area under the Betti curve. The results show a coherent difference across topological dimensions: similar words generate stable connected components with lower variability, while dissimilar words produce a richer set of cycle features that persist across a broader range of scales. These findings indicate that persistent homology can capture multi-scale structural differences in embedding spaces that are not visible through standard distance-based comparisons. Although the experiment is intentionally simple, it highlights the potential of topological methods for studying how semantic structure is distributed across levels of a neural embedding space.

Keywords: TOPOLOGICAL DATA ANALYSIS, PERSISTENT HOMOLOGY, SENTENCE EMBEDDINGS, SEMANTIC SIMILARITY, SYNONYMS AND ANTONYMS, NATURAL LANGUAGE PROCESSING;

1. Introduction

Word meanings are rarely isolated. Some words share almost the same meaning, others express the exact opposite, and many are simply unrelated. Modern language models try to capture these relationships by representing words or sentences as points in a high-dimensional space called an embedding space. If two meanings are close, their vectors should also be close; if they differ strongly, they should drift apart. While this idea is intuitive, the actual structure of such embedding spaces is still not fully understood.

Topological Data Analysis (TDA) offers a way to look at the global shape of a dataset rather than only pairwise distances or statistical averages. Persistent homology, one of the core tools in TDA, can detect patterns such as clusters, loops or fragmentation that may not be obvious from direct numerical comparisons. Its main advantage is stability: small changes in data usually do not destroy the overall topological signal.

There have already been attempts to apply TDA to text data, mostly in the context of large corpora or document classification. These studies show that topological descriptors can sometimes reveal hidden structures or improve machine learning tasks. However, much less is known about how basic semantic relationships, like synonymy or antonym, appear from a topological perspective. In other words, does the *shape* of an embedding set change depending on the type of meaning relation?

The aim of this paper is to explore this question in a simple and controlled way. Instead of working with a large or noisy dataset, we focus on a small subset of word pairs taken from the SimLex-999 benchmark. The dataset allows us to separate pairs with high similarity scores from those with very low similarity. For each word, we generate short template-based sentences, embed them using a transformer-based model, and compute persistent homology on the resulting point clouds.

Our goal is not to build a classifier or prove superiority of one embedding method over another. Rather, we want to see whether the topological signatures of the two groups differ in a consistent way. As the results will show, high-similarity pairs tend to form more compact structures with shorter persistence, while low-similarity pairs exhibit more spread and higher complexity. Although preliminary, these findings suggest that topology can provide a different viewpoint on how meaning is encoded in modern embedding models.

2. Related work

Topological Data Analysis has become a useful tool for studying complex, high-dimensional datasets, where traditional geometric or statistical methods struggle to capture global structure. A key milestone in the development of persistent homology as a computational framework was the work by Zomorodian and Carlsson, who formalized how topological features can be detected and tracked across different spatial scales [1]. Later, Adams et al. introduced persistence images, offering a stable and vector-based representation of persistence diagrams suitable for machine learning workflows [2]. These foundations make it possible to analyze embedding spaces not only by distance, but also by their structural and topological properties.

The idea of applying persistent homology to natural language data is relatively recent. One of the first steps in this direction was taken by Fontana et al., who explored whether word embeddings contain detectable topological patterns and showed that such patterns can be used as features in text classification tasks [3]. While their work demonstrated feasibility, it focused on downstream prediction rather than understanding how specific semantic relationships appear in embedding space.

To evaluate semantic similarity more explicitly, benchmark datasets such as SimLex-999 were introduced, providing human-judged similarity scores that allow systematic comparison of word meaning [4]. Alongside this, new embedding models such as Sentence-BERT have made it possible to generate meaningful sentence-level representations while preserving relational structure between words and phrases [5]. More recently, research has shifted toward studying the global behavior of embedding spaces themselves. For example, De Silva et al. showed that persistent homology can reveal structural differences between embedding spaces, such as non-isometric distortions across languages or models [6].

Although these studies point toward the usefulness of topology in language representation research, there is still limited work on controlled experiments that focus specifically on semantic relations. The present paper addresses this gap by analyzing whether persistent homology can reveal measurable differences between embeddings of highly similar versus weakly related word pairs.

3. Methodology

3.1 Dataset and Sentence Construction

When introducing a dataset into a project, it is of crucial importance to have it well organized, especially when working with topology, where everything can be viewed and presented in different ways. In our case, we take word pairs and introduce them into context-independent sentences, which will later be embedded and topologically analyzed.

As the basis of this experiment, we decided to use the SimLex-999 dataset, which is composed of 999 pairs of words. The pairs can consist of abstract adjectives, nouns, or verbs, where each pair is graded according to how similar the words are. Words with related meanings (synonyms) are graded higher, while words with opposite meanings are graded lower.

Besides SimLex-999, there are other datasets as well, such as WordSim-353 and MEN, which, in contrast to the dataset used in this work, grade the meaning only between two nouns and their association. These differences can lead to divergent results, which opens new possibilities for the future, but for now we decided to continue with SimLex-999, as it provides more appropriate data for our needs.

For this experiment, we separated the 999-word pairs into two subsets. First, the dataset was sorted by the similarity score and then split in half:

- 0.23 – 4.67: group with lower semantic similarity
- 4.68 – 9.80: group with higher semantic similarity

This separation allowed us to perform a controlled analysis and comparison between these groups and their semantic behavior.

Since isolated words cannot provide sufficient information about their usage or contextual nature, every word was integrated into context-independent sentences. These types of sentences are of a good value because they retain their semantic structure regardless of which word is inserted into them.

The decision to use these types of sentences allows us to examine the dependency between words with high semantic similarity and those with low similarity, as well as to observe their behavior in these controlled contexts.

Each of the 1,998 words was inserted into ten different template sentences, resulting in a total of 19,980 sentences. This enabled us to observe the behavior not only of the individual words but also of the words within full sentence contexts, which is a significant factor for the subsequent topological and embedding analysis discussed in the next section.

3.2 Sentence Embeddings and Point-Cloud Construction

After constructing the full set of generated sentences, the next step was to convert them into numerical representations that could be meaningfully compared. For this purpose, the Sentence-BERT AllMiniLM-L6-v2 model was used as the embedding engine. This model is widely used because it produces semantically meaningful sentence-level embeddings without requiring task-specific fine-tuning.

In practice, the model takes each sentence and maps it to a fixed-dimensional vector:

$$x = E(s) \in \mathbb{R}^{384}$$

Each embedding can be interpreted as a coordinate in a 384-dimensional semantic space. Because differences in magnitude are not informative for this analysis, all vectors were normalized to unit length using:

$$\hat{x} = \frac{x}{\|x\|_2}$$

Once normalized, the cosine similarity between two embeddings simplifies to a distance measure based purely on the angle between them. In this form, Euclidean distance and cosine similarity are interchangeable, and distance can be expressed as:

$$d(\hat{x}_i, \hat{x}_j) = 1 - \langle \hat{x}_i, \hat{x}_j \rangle$$

With the embeddings computed and normalized, the next step was to apply PCA, reducing their dimensionality from 384 to 150. This reduction decreased the computational cost, enabling faster execution and lower energy consumption.

As we previously discussed, from there they were grouped according to their source word's similarity classification from SimLex-999. This created two distinct and balanced point sets:

$$X_{HS} = \{\hat{x}_1^{HS}, \dots, \hat{x}_{999}^{HS}\} \quad X_{LS} = \{\hat{x}_1^{LS}, \dots, \hat{x}_{999}^{LS}\}$$

Each sentence embedding corresponds to one point in the space, meaning each group forms a point cloud. Conceptually, these clouds represent how the model organizes meaning internally.

3.3 Persistent Homology Analysis

To move beyond pairwise distances and explore the shape of the embedding space, persistent homology was applied. Unlike standard clustering or dimensionality reduction methods, persistent homology does not rely on assumptions about convexity, density, or linear separability. Instead, it examines how connectivity patterns evolve across distance scales and records geometric structure that remains stable across those scales.

The analysis begins by constructing a Vietoris–Rips filtration, which builds a family of simplicial complexes based on a threshold parameter ε . For a given value of ε , a simplicial complex is defined as:

$$VR_{\{\varepsilon\}}(X) = \{\sigma \subseteq X \mid d(x_i, x_j) \leq \varepsilon, \forall x_i, x_j \in \sigma\}$$

At $\varepsilon = 0$, every point is isolated. As ε increases, points connect into edges, triangles, and higher-order simplices, eventually forming a fully connected structure. Persistent homology tracks when these structures appear (their birth) and when they vanish (their death).

For each topological dimension k , this process produces a set of birth-death intervals:

$$D_k = \{(b_i, d_i), i = 1, \dots, N_k\}.$$

In this work, only the first two dimensions are examined:

$k = 0$: connected components, representing how quickly points merge into clusters.

$k = 1$: loops or cycle structures, which suggest curved or hollow regions in the cloud.

To compare the two point clouds quantitatively, several commonly used persistence-based descriptors were computed. The first was the average lifetime of features:

$$\bar{L}_k = \frac{1}{N_k} \sum_{i=1}^{N_k} (b_i - d_i)$$

which serves as a measure of how long topological features persist before collapsing.

A second descriptor was persistence entropy, which captures how evenly or unevenly feature lifetimes are distributed:

$$p_i = \frac{d_i - b_i}{\sum_{j=1}^{N_k} (d_j - b_j)} H_k = - \sum_{i=1}^{N_k} p_i \log(p_i).$$

Finally, Betti curves were generated to provide a scale-dependent view of topological structure:

$$\beta_k(\varepsilon) = |\{(b_i, d_i) \in D_k | b_i \leq \varepsilon < d_i\}|$$

4. Results

Persistent homology was computed separately for the high-similarity and low-similarity groups of sentence embeddings. For each filtration, birth–death intervals were extracted and summarized using the average lifetime, the persistence entropy H_k , and the area under the Betti curve AUC_{β_k} . All numerical descriptors are reported in Table 1.

Table 1 The results for average lifetime, entropy and Betti AUC

		$\bar{L}_k$	$entropy_k$	AUC_{β_k}
High similarity, $k = 0$		0.547886	8.874602	1901.88
		0.357307	9.129177	1579.12
Low similarity, $k = 0$				
High similarity, $k = 1$		0.099668	7.013554	417.92
		0.185433	9.057350	497.34
Low similarity, $k = 1$				

For dimension $k = 0$, which reflects the merging of connected components, the high-similarity group exhibits a larger average lifetime ($\bar{L}_0=0.547886$) compared to the low-similarity group ($\bar{L}_0=0.357307$). This indicates that components in the high-

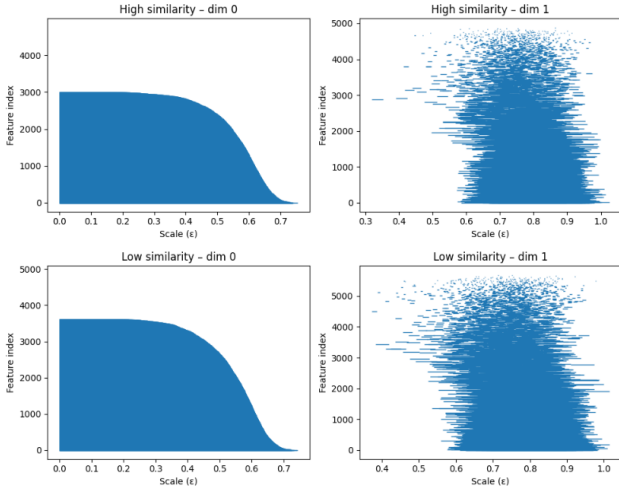


Figure 1 Persistence Barcodes for High-similarity and Low-similarity group

similarity embedding cloud persist over a wider range of scales before merging. The corresponding entropies show the opposite trend: the low-similarity cloud exhibits a higher entropy value ($entropy_0=9.129177$) than the high-similarity cloud ($entropy_0=8.874602$), suggesting that lifetimes in the low-similarity group are more dispersed and heterogeneous. The Betti AUC values follow the same pattern ($AUC_{\beta_0}=1901.88$ vs. $AUC_{\beta_0}=1579.12$).

For dimension $k = 1$, which captures loop-like configurations, the differences are more pronounced. The low-similarity group shows a larger average lifetime ($\bar{L}_1=0.185433$) than the high-similarity group ($\bar{L}_1=0.099668$), meaning that cycles in the low-similarity cloud persist across a broader part of the filtration. The entropy values are again higher for the low-similarity group ($entropy_1=9.057350$ vs. $entropy_1=7.013554$). This is reflected in the Betti AUC values ($AUC_{\beta_1}=497.34$ vs. $AUC_{\beta_1}=417.92$). The persistence diagrams are shown in Figure 1.

Taken together, these observations show a consistent pattern across dimensions. Semantic similarity produces longer-lived components with lower variability, while lower similarity yields shorter component lifetimes but longer and more heterogeneous cycles. Even though sentences were generated using a fixed template, persistent homology detects differences in the geometry of the embedding space.

5. Discussion

The results suggest that semantic similarity shapes the topology of the embedding space in two complementary ways. At small filtration scales, the embeddings of sentences built around closely related words tend to remain separated for longer and collapse into connected components in a more uniform fashion. This behavior is reflected in the higher average lifetime $\bar{L}_0$, lower persistence entropy, and a larger AUC_{β_0} for the high-similarity group. Since the sentence template was identical across all samples, the only source of variation was the target word inserted into the sequence. The stability of these small-scale features therefore points to a genuine effect of semantic coherence: similar concepts induce tighter local neighborhoods in the model's latent space, and their merging across scales follows a more stable trajectory.

At larger scales, the situation reverses. Embeddings derived from sentences containing dissimilar words produce richer and more sustained loop-like configurations, captured by longer average lifetimes $\bar{L}_1$, higher entropy, and a larger AUC_{β_1} . These signatures indicate that the low-similarity point cloud spans a broader portion of the embedding manifold, creating intermediate gaps that take more time to fill during the filtration. In this case, the absence of semantic coherence does not simply produce random noise; instead, it seems to encourage exploration of directions that unfold into higher-order geometric structure. The difference between the two scenarios aligns with an intuitive interpretation of how deep language models organize meaning: clusters form readily around coherent concepts in local neighborhoods, while global manifold structure emerges from contrasts between unrelated semantic axes.

From a methodological perspective, the coexistence of these two effects is significant. Classical embedding analyses often rely on clustering, dimensionality reduction, or cosine similarity comparisons. While such tools can reliably capture local coherence and relative distances, they provide limited information about how structure evolves across scales. Persistent homology offers a complementary view: the transition from isolated components to higher-order simplices is tracked throughout the filtration, making it possible to evaluate not only whether two concepts are close but also how their neighborhoods merge and what features arise along the way. In this experiment, the topological descriptors captured differences that cannot be reduced to a single similarity score, showing that topology can reveal both stability within semantic clusters and variation driven by conceptual diversity.

The patterns observed in the diagrams and summary metrics are also consistent with the geometric behavior of deep language models such as BERT. These models embed linguistic information on a non-linear manifold, where semantic directions do not align to simple axes but arise from a training signal distributed across multiple layers. As a result, a group of sentences containing similar words may form a compact region supported by shared contextual structure, while diverse concepts generate a broader arm of the manifold that wraps around pre-existing clusters. The persistence of 1-dimensional features in the latter case suggests that the global geometry has curvature and gaps that require multiple filtration thresholds to close. This perspective emphasizes the relevance of topological tools for understanding latent spaces shaped by implicit tasks and unsupervised objectives.

Finally, it should be emphasized that these findings arise from a controlled and deliberately simple setting. The sentences were generated using an artificial template, and only one word varied across samples, making this a highly constrained experiment. This setup allowed the effect of semantic similarity to be isolated, but it does not capture the full richness of natural language, nor does it explore how topology behaves under different syntactic constructions, sentence lengths, or contextual structures. The present study illustrates a single experiment designed to highlight the presence of topological signatures rather than to provide comprehensive statistical conclusions.

6. Conclusion

This work explored whether topological features derived from sentence embeddings reflect differences in semantic similarity between words. By constructing controlled sentence templates and applying persistent homology, we obtained a geometric view of the embedding space that goes beyond pairwise distances. The results show that the two groups of sentences produce distinct patterns. Their persistence descriptors and Betti curves, indicating that semantic similarity influences the structure of the point cloud at multiple scales. Although the experiment is intentionally simplified, the observations suggest that topological summaries may serve as a complementary way to characterize embedding behavior.

7. Future work

This study highlights a clear topological signal associated with semantic similarity, but several directions remain open. A natural extension is to move beyond synthetic sentences and apply the same analysis to real text corpora, where variation in sentence structure, context, and discourse patterns may produce richer and less predictable geometric behavior. In particular, persistent homology could be applied to document-level embeddings, contextualized sentence embeddings, or token-level trajectories across layers of a transformer model.

A second line of investigation concerns the embedding models themselves. The present experiment used a single encoder architecture, and it is not yet known whether the observed patterns generalize across different model families, such as BERT variants, sentence-transformers, large decoder-based models, or multilingual encoders. Comparing the topological signatures across architectures could clarify whether cycles and component persistence arise from general properties of modern language representations or from model-specific inductive biases.

Third, the current work employed a Vietoris–Rips filtration on the Euclidean metric. Alternative filtrations such as, witness complexes, or density-based filtrations may highlight different aspects of the underlying geometry and help distinguish between noise-driven features and persistent structures. In addition, the use of persistence landscapes or kernel-based methods may enable statistical testing on collections of diagrams rather than relying on single-instance descriptors.

Finally, a larger-scale study could explore connections between topological descriptors and downstream tasks. If persistent features correlate with clustering quality, classification performance, or interpretability measures, then persistent homology could play a practical role in model diagnostics. More broadly, the topological approach may offer an avenue toward explaining how semantic information is organized in embedding spaces, complementing existing explainable AI techniques that focus on feature importance or attention patterns.

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