CONTRIBUTIONS TO THE OPTIMIZATION OF PELLETS AND BRIQUETTES MANUFACTURING PROCESSES USING ELEMENTS OF ARTIFICIAL INTELLIGENCE, STATISTICS AND OPERATIONAL RESEARCH

PhD thesis – Abstract

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author Mariș Simina-Ștefania
doctoral advisor Prof.univ.dr.ing. Titus Slavici

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INTRODUCTION

Pellets and briquettes are produced by mechanical agglomeration or pressing of the raw material, after it has been previously crushed or powdered, for transport, further processing or use.

In this paper, the pellets and briquettes for heating will be studied and the main original results obtained will be presented. The importance and necessity of the topic, the research objectives and the structure of the paper will be further detailed.

Importance and necessity of the topic

Energy is a key component of the current progress and development of civilization. Among the biomass processing technologies in order to obtain energy, pelletizing and briquetting have an increased efficiency. These technologies make it possible to significantly reduce the volume of biomass, as comfort of use increases [3].

Given the huge potential of solid fuels obtained from biomass, both in terms of energy input, but also in terms of ecology and sustainable development, this field of production is strongly supported at European and regional level.

Starting with the second half of the twentieth century and with the development and widespread use of computers and the development of information technology, the processes specific to industrial engineering began to be redesigned. By using experimental design techniques, modelling techniques and numerical simulation software, the costs of the experimental research required to improve production can be reduced.

The current work uses elements of information technology (in particular programming and artificial neural networks) to predict and optimize the processes that occur in an enterprise whose main object of activity is the manufacture of pellets and briquettes from wood waste, used as alternative energy source.

Objectives of the research

The optimization of the manufacturing process of pellets and briquettes for heating can refer to maximizing profit, increasing productivity, recycling waste of agricultural or forestry origin, maximizing calorific value, compliance with technical standards, determining production recipes specific to each of these cases, to innovative solutions for automation of the production line, etc. These aspects will be detailed in this thesis.

The primary objectives to be achieved during the doctoral research internship are:

OP1 obtaining scientific and technological results on the use of renewable natural resources for the production of pellets and briquettes

OP2 optimization of recipes for the manufacture of pellets and briquettes from various research directions using industrial scientific planning and research

In order to achieve the primary objectives, it is necessary to achieve the following **secondary objectives**, corresponding to the activities carried out in this research stage:

OS1 design of experimental activities and development of a methodology for conducting experimental research

OS2 proposal for improvements in the production process

OS3 creation of a dynamic system of know-how applicable in several directions

OS4 development of a software for forecasting calorific value, pollutants and costs in the case of various innovative products such as renewable energy

Structure of the thesis

The paper is structured in 7 chapters. The approach of the research specific to this thesis begins with the presentation of a company that produces pellets and briquettes for heating. Solutions are identified for its modernization and for the innovation of production lines. Within the production lines, pellet recipes made with materials from the area are realised and, through their analysis, improved recipes are determined, which are characterized by high calorific value and low percentage of residual ash. New directions of research and diversification of production are identified. Since determining a pellet recipe that maximizes calorific value while the amount of residual ash and pollutants falls within certain limits is a problem of linear optimization, the next logical step was to mathematically describe this problem and study the existence of the solution and its properties. A database was created with properties of the main materials available for pellet production and, associated with it, a software solution for determining a recipe with several components based on the solution of the linear optimization problem. The existing database can be completed by the user either on the basis of direct experimental determinations or by a hybrid method (the use of a neural network to supply the necessary data that cannot be determined experimentally).

1 CURRENT STATE OF RESEARCH IN THE TOPIC OF THE PROPOSED THESIS

Given the complexity of the topic, the current state of research can be considered from several points of view as follows:

- in terms of renewable energy production using solid biofuel and reference data currently applicable in the production of pellets and briquettes for heating
- in terms of the use of linear programming techniques in production
- in terms of the use of neural networks and algorithms specific to artificial intelligence for determining and completing certain data
- in terms of the feasibility of a technology transfer

All these points of view will be detailed below, in order to achieve a more accurate image of the current state of research in the field.

1.1 Trends and benchmarks in the production of solid renewable biofuels

The possibility to use wood or agricultural waste efficiently for energy production is a current trend in both industry and household consumption.

Standards, physico-chemical characteristics, production and logistics data, combustion technologies, cost analysis for both production and use of pellets for heating, an analysis of the environmental impact and also a market analysis for pellets were collected and presented in 2010 by Obernberger and Thek [18]. The specifications of solid biofuels such as pellets and briquettes are subject to standards that are constantly updated. EU regulations for these types of biofuels are included in the standards EN 17225-1 [4], EN 17225-2 [5] and EN 17225-6 [6]. From this point of view, the following standards are accepted:

- standards for wood pellets and briquettes for domestic consumption: Enplus A1, Enplus A2, Enplus B
- standards for wood pellets and briquettes for industrial consumption: I 1, I 2, I 3
- standards for pellets and briquettes from non-woody biomass and biomass blends: MBP A, MBP B

Given the current global needs and problems in the field of energy [10] as well as the new development opportunities in the field of renewable energies in Romania, a new direction in the field of industrial research and development is logically outlined. This refers to the determination of techniques for optimizing the processes associated with the production of biofuels.

Determining the calorific value for various solid biofuels has always been a challenge. Relevant papers in this field in the context of the thesis include [11], [12], [14], [19].

Current trends in the use of linear programming techniques in production

Linear optimization (or linear programming) is a mathematical method of determining an optimal value under certain conditions that is used in project selection, production planning, mixtures of certain products, etc. Determining a mixture of two types of biomasses to maximize calorific value while the noxious elements in the chemical composition remain below the permissible limit values leads to the determination of the solution of a linear optimization problem.

Current trends in neural network applications

A reference for any work that addresses issues related to artificial intelligence is the work of Russell and Norvig [21]. A well-known software for building and analyzing neural networks is Matlab. In [17] Demuth and Beale present, in addition to the fields in which neural networks built with Matlab and neural models can be applied, network architectures, training functions, back-propagation algorithms, etc.

Current trends in technology transfer and their importance for innovation

There is a strong connection between research and applied research. Over the last century, innovation has gradually become the most important factor in increasing productivity. Consequently, the role of academic research and its applications in socio-cultural and economic development can no longer be denied.

Technology Readiness Level (TRL) refers to the stage of development of that technology. The readiness level increases from 1 to 9 as follows:

- Levels 1-3 (TRL 1 – TRL 3) are the research phase
- Levels 4-6 (TRL 4 – TRL 6) constitutes the development phase
- Levels 7-9 (TRL 7 – TRL 9) constitutes the implementation phase

1.2 Framing the research in the current state of knowledge

Innovation, like any other human activity, requires an input of energy, which must be produced using existing resources (either conventional or unconventional resources). The concern for a better use of energy resources is very topical, both at European and national level.

This thesis analyses various types of biomasses that can be used in the production of pellets and briquettes for heating, but without going into details on the markets. By analysing the research in the field (for example [18]) the importance of using an additive in the pelletizing process was revealed.

By analysing the possibilities of applying linear programming techniques to optimize the manufacturing process of heating pellets, along with research trends in this field, the objective function to be optimized was identified as the calorific value of a mixture of several raw materials, and for the constraints - the emitted noxious substances and the amount of residual ash resulting from combustion. The maximum values for these constraints are in principle determined by the maximum values allowed in the standards.

We are not aware that this technique has been applied in the past to determine an optimal biomass recipe (for which the maximum calorific value is obtained when the value of the noxious substances remains below a certain level).

We preferred to study the relationship between the elemental composition of the raw material, on the one hand, and the calorific value, and the amount of residual ash resulting from combustion, on the other hand. Given that the accuracy of the trained network exceeds 90%, the choice of one of the two sets of inputs (plus the related outputs) available depends exclusively on the possibility of performing physico-chemical analyses on raw materials.

An integral part of the efforts to improve Romania's innovation capacity, this research aims to contribute to increasing cooperation between academia and the industrial sector by achieving a viable technology transfer. The elements of theoretical research in the field of operational research will be validated experimentally first at the laboratory level and then in an enterprise, in order to contribute to the increase of its competitiveness.

The original, novel elements that are the subject of this paper have the effect of reducing research costs for companies that produce pellets and / or briquettes from biomass, while increasing the quality of production.

2 CONTRIBUTIONS TO THE OPTIMISATION OF THE ARCHITECTURE OF A TECHNOLOGICAL LINE FOR THE PRODUCTION OF PELLETS AND BRIQUETTES

The objectives of this chapter are:

- presentation of a typical technological line for the production of pellets and briquettes, functioning in a specialized micro-enterprise
- presentation of a solution for optimising the technological line for the production of pellets and briquettes from biomass mixtures
- identifying solutions for financing investments in such a company

The original results of this research chapter are:

- a scheme for a technological line optimized for the production of pellets from mixtures
- two project drafts for accessing European funds

2.1 The classic concept of technological lines for the production of pellets and briquettes

The process of transforming the raw material into pellets or briquettes has several stages:

- feeding stage (includes sorting, chopping and refining the raw material)
- drying stage (in which the raw material is brought to the required humidity)
- the pelletizing or briquetting stage itself
- cooling stage of the finished product
- packing stage

Initially, the technological line consisted of the following essential components for the operation of the factory: shredder, hammer mill, drying plant, press hopper, pellet press, briquette press, sieve screening and pellet cooling.

For the briquetting line, the feeding and drying stages use the same equipment. A hydraulic piston lighter press is used for pressing.

2.2 Optimization scheme of the technological line for pellets

By analysing the technological processes necessary for the production of pellets, as well as the possibilities of using the available raw material, was highlighted the need to complete the technological line with elements that allow the simultaneous processing of several raw materials for palletisation, but also elements that allow production in small series, for experimental testing and validation of research results.

At least the following additional equipment is required to perform the experiments:

- sieves and moulds of various sizes for the hammer mill and pellet press
- a second shredder, to be able to process two types of biomasses simultaneously
- a second hopper to store two types of biomasses simultaneously
- a mixer for making mixtures of at least two components
- small capacity pellet press (hobby press) to test the obtained recipes

With the hobby press, the pellet recipes studied in the thesis were made.

2.3 Solutions for financing the development of technological lines

For the development of technological lines, the best option is to use European funds. Without going into details, the following will illustrate how these funds can be used to improve the production lines.

Financing through STARTUP NATION type projects

The Start-up Nation program is a program designed to encourage and stimulate the establishment and development of small and medium-sized enterprises. Through this project, the start-up wants to acquire a technological line for processing pellets and briquettes.

The long-term goals assumed by the start-up are correlated with the desired investment. As a result of the implementation of this project is the obtaining of an optimized technology for the production of pellets and briquettes, both from the point of view of the composition of the biomass mixtures used, and from the point of view of the working regimes of the machines.

The SWOT analysis highlights process innovation as the main strengths, identifies the main opportunities as coming from the growing demand for developed products.

The activities of the project and the equipment to be purchased for these activities are described, an analysis of the market for heating pellets is carried out and a budget for procurement is proposed.

Figure 2.1 Small capacity pellet press operation detail

Financing through the Competitiveness Operational Program (Programul Operațional Competitivitate)

Another method to finance a start-up in the field of renewable energy production is through the Operational Program Competitiveness, action 1.2.1, through projects such as "Innovative start-up and spin-off enterprises".

This type of projects is aimed at innovative start-ups or spin-offs and their main focus is on the development and marketing of significantly improved products or technologies. Through this program, a non-reimbursable financial assistance of maximum 840,000 lei (equivalent to 200,000 Euros) is granted, representing 90% of the total eligible costs of the project, the remaining 10% of these costs being borne by the beneficiary. A project can take up to 2 years.

One of the specific objectives of the project is to create an innovative recipe for the manufacture of pellets and / or briquettes, from various directions of research through the recovery of forest and agricultural residues.

The activities proposed to be carried out within the project are: research and development activities (industrial research and / or experimental development), procurement of research and development services, activities for introduction into production and product / process / technology realization, procurement activities of raw materials and materials necessary for the realization of the project, information and publicity activities regarding the project, activities to ensure visibility, activities for project management and audit.

This project was submitted in 2017, has been won and is being implemented.

3 THEORETICAL FUNDAMENTALS OF RESEARCH

The objectives of this chapter are:

- theoretical foundation of the research
- review of the various techniques of fundamental research [20], [25], [21] that will be used in the following chapters

General information on the organization of experimental research and the scientific planning of factorial experiments, experimental data processing techniques, elements of operational research and artificial intelligence, as well as the dedicated software Statgraphics Centurion and Matlab, used in the thesis to obtain specific results, will be reviewed.

3.1 Overview of the organization of experimental research on the line of pellets and briquettes

Each research activity is based on previously collected data. Measuring a physical quantity means comparing it to another physical quantity, called a standard or unit of measurement, using a particular principle (or method) of measurement. Any measurements are affected by errors - random, systematic or mistakes.

A statistical method of analyzing measurement data that depends on one or more factors with simultaneous action, in order to establish their significance on the objective function is dispersional analysis (or analysis of variance).

After determining a theoretical model for a process or phenomenon, it will be simulated. The simulation is done using programming techniques and aims to study the process or phenomenon analyzed in certain circumstances, which can be controlled by the user. By varying the parameters, the user can form an overview of the phenomenon studied, can understand it, can study it using available resources [83].

3.2 Considerations for the scientific planning of factorial experiments

Experimental design (scientific planning of experiments) is a rigorous and systematic approach to the problem-solving process [17]. Through this, in the stage of collecting experimental data, various principles and techniques are applied in order to ensure valid and consistent conclusions with the lowest possible consumption of resources.

3.3 3.3 Experimental data processing techniques

Traditional statistical methods used to link input data with output data are generally called "curve fitting" (whether they refer to interpolation or regression).

The most commonly used regressions are linear regression (which determines a line as the best approximation of a scatter plot), nonlinear regression (which determines a curve as the best approximation of a scatter plot) and multiple regression (in which case the dependent variable depends on several independent variables).

The approximation error depends on a number of factors that are more or less controllable in practice, such as the degree of homogeneity of the analyzed sample or the accuracy of the measurements [17]. One of the most commonly used methods for determining regression equations is the least squares method.

Any model for which the coefficients can be converted into linear coefficients can be reduced to a linear model. The main characteristics of the regression equations are the correlation coefficient, the standard deviations and errors, the coefficients of determination.

Aberrant values are those values that do not fit into the general pattern of other values. In the case of a normal distribution, the rule of thumb is that the value deviated from the mean by more than 3 standard deviations is an aberrant value. Aberrant values can greatly influence the regression coefficients, so it is important that they are identified [17], [2] and eliminated.

3.4 Statistical data processing using Statgraphics Centurion

Statgraphics Centurion XVI is a software for statistical data processing, developed by StatPoint Technologies [23] and was the first software for statistical analysis adapted for use on personal computers, the first software that used graphical methods to illustrate statistical data.

The data is entered into a so-called Data Book, organized similar to an Excel worksheet, in which each column corresponds to a specific piece of information to analyse. To analyse them, you can choose the desired procedure from the main menu or the menu bar, or you can use the built-in wizard, StatWizard.

3.5 Elements of operational research applicable to research

Operational research is a branch of applied mathematics that deals with the creation and application of analytical methods that allow an improvement of the decision-making process. In this way, optimal solutions are found for complex problems involving decision-making.

The steps to solve a problem with the help of operational research are [1]:

1. defining the problem
2. classification and conceptualization of the problem
3. formulation and construction of the mathematical model
4. the solution of the model, which provides feedback on the conceptualization process
5. validation, sensitivity analysis and recommendations
6. if the solution is applicable, it will be implemented.

A linear programming problem (or linear program) usually takes the following form [1]:

find the maximum (or minimum) of an objective function

$$f(x_1, \dots, x_n) = \sum_{i=1}^{n} c_i x_i \tag{3.1}$$

given the constraints

$$\sum_{i=1}^{n} a_{ji} x_i \leq b_j \quad , 1 \leq j \leq m \tag{3.2}$$

A solution to the linear programming problem consists of those x_i values that verify the constraints.

Any linear optimization problem can be brought to a standard form, which is solved using the simplex algorithm.

Theorem [25] If the program in standard form (P) is compatible and all its basic admissible solutions are undegenerated then the application of the simplex algorithm ends in a finite number of iterations, either with finding the optimal solution or with the conclusion that the program has optimal infinite.

3.6 Artificial intelligence methods in process optimization and prediction

Artificial intelligence (AI) is the intelligence demonstrated by machines. Among its elements, artificial neural networks (ANN) began to be used extensively since the 1980s. ANN "neurons" are software elements that simulate human neurons. In principle, a neuron is composed of an input, p, transmitted through a connection that multiplies its power by the weight w, a transfer (or activation) function $f\ (wp)$ and an output a. A threshold (bias or displacement), b, it can be assimilated to an input equal to the unit and a weight b. The output of the neuron will thus become $a = f\ (wp + b)$.

The structure of a forward-propagating RNA consists of:

- an input layer - I, containing a certain number of neurons,
- one or more hidden layers - H (each composed of a certain number of neurons)
- an output layer - O, usually composed of a single neuron (the “response” of the network).

ANN find applications in all fields: financial-banking, insurance, aerospace, automotive, defense, electronics, entertainment, industry, manufacturing, medicine, robotics, speech and writing recognition, security, telecommunications and even estimating gross calorific value.

3.7 Design of neural networks using Matlab

One of the most used software solutions for the implementation of neural networks is Matlab [13][17].

In order to use ANN, the following steps must be followed:

- the training stage (in which the known associations between inputs and outputs are introduced in the network);
- validation stage (in which the ANN results are verified by comparison with known results);
- testing stage (in which the ANN predicts results associated with input data sets).

The standard training algorithm for a forward propagation network is the backpropagation algorithm, which aims to minimize an error function. Basically, the error function measures the performance of the network.

Two of the most important problems of backpropagation are the low convergence rate and the limited ability to generalize. The low speed of convergence (the fact that the error decreases too slowly) can be remedied using fast algorithms, based on heuristic techniques (such as variable speed feedback), or numerical optimization techniques (such as conjugate gradient method, quasi-Newton method, Levenberg-Marquardt). An improvement of the generalization capacity can be obtained using either the Bayesian regularization method (which operates at the level of the error function) or the early stop criterion (when the network drive algorithm is not one that converges quickly).

4 EXPERIMENTAL RESEARCH ON HEATING PELLETS. PROCESSING AND INTERPRETATION OF OBTAINED DATA

The objectives of this chapter are:

- To establish a methodology for experimental research on heating pellets
- To conduct field experiments in order to determine the properties of pellets for heating and their analysis
- To determine of a pellet recipe that maximizes the calorific value (in MJ / kg) when using the main raw materials available in the area, when the residual ash falls within the limits of a certain standard or is minimized
- To study of the influence of an additive on the quality of the final product (calorific value, ash, homogeneity, density)
- To identify related research directions for the diversification of production
- To perform a preliminary qualitative study of the potential of willow bark

The original results obtained are:

- a methodology of research
- a series of pellet recipes for local raw materials, with or without additive
- pellet samples made with the proposed recipes
- an estimate of the properties of the pellets obtained from raw materials in the area (in terms of calorific value and residual ash, compliance with standards) according to the manufacturing recipe

- a series of formulas that predict the quality of pellets from fir sawdust and wheat grains depending on the amount of additive (corn grains) added
- an initial qualitative study of the possibilities to diversify production
- a preliminary estimate of the amount of salicin that can be obtained by separately processing the willow bark

4.1 Methodology of experimental empirical research by decomposition into primary chemical elements

In the following, the key concepts used in this chapter in experimental empirical research will be presented, as well as the main methods and equipment used in research (a research methodology, methods of analysis of results).

Humidity is defined as the total amount of water, as a percentage, present in the fuel.

Ash is the solid residue that remains after burning the fuel to a constant mass at temperatures of $815^o \pm 25^o$ [24].

Lower calorific value (also known as useful calorific value or industrial calorific value) is defined as the amount of heat released by the "perfect and complete" combustion of a mass unit of a given fuel when water vapours are not condensed and the latent heat of vaporization does not recover.

Particle density is a factor that influences the quality and burning time of pellets. Closely related to particle density is the bulk density of pellets.

The key concepts, which are detailed in the thesis, refer to:

A. Establishing a working methodology
B. Determining the lower calorific value
C. Determining the residual ash
D. Determining the geometrical parameters for the pellets

4.2 Determination of calorific value and residual ash for mixtures

In order to determine the calorific value and residual ash, a first step is to define an experimental strategy. After the actual realization of the experimental determinations, the collected data are analysed and interpreted with the help of Statgraphics Centurion.

Experimental strategy

The aim of the experiment is to determine the influence of pellet composition on calorific value and residual ash, in the case of mixtures of up to 5 components, among the most common raw materials in the Eastern European plain area.

A linear model was chosen for the composition of the mixture, the factors of the experiment being A (straw), B (beech sawdust), C (chopping / branch residues), D (non-compliant corn grains), E (non-compliant wheat grains). The 5 types of raw material and the pellets obtained from them are presented in Figure 4.1.

Effective realization of experimental determinations

For each mixture of the 15 proposed for analysis, pellet samples were made at the Cenei factory and were further analyzed in the Research Center for Machines and Thermal Equipment, Transport and Pollution Control at the Polytechnic University of Timisoara.

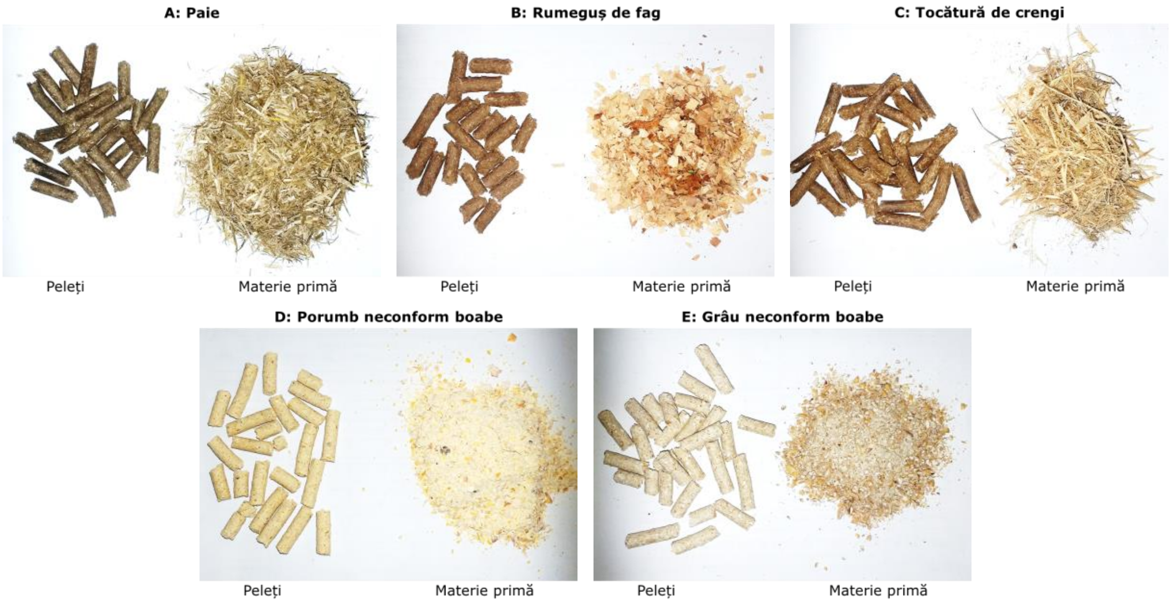

Figure 4.1 Experimental factors (raw material and pellets)

Evaluation of the experiment, analysis and interpretation of the data obtained

The analysis of the mixture indicates that the model that best describes both the calorific value of the mixture and the percentage of residual ash is a linear model.

The regression model for calorific value is

$$Q = 15{,}9299 \cdot Factor_A + 18{,}7661 \cdot Factor_B + 18{,}375 \cdot Factor_C + \\ + 16{,}9027 \cdot Factor_D + 16{,}2113 \cdot Factor_E \quad (4.1)$$

with the constraint that the sum of the factors must be equal to 1 (100%). This model explains 100% of the variation in calorific value. The standard estimation error is 0.000338062, and the mean square deviation is 0.000228571. The maximum value for Q is 18.77 (corresponding to the case where the mixture is made entirely of beech), and the minimum is 15.93 (corresponding to the situation where the mixture is made entirely of straw).

The regression model for the ash is

$$ash = 4{,}26133 \cdot Factor_A + 2{,}17048 \cdot Factor_B + 2{,}01762 \cdot Factor_C \\ + 0{,}729048 \cdot Factor_D + 2{,}28819 \cdot Factor_E \quad (4.2)$$

with the restriction that the sum of the factors must be equal to 1 (100%).

The minimum value for residual ash is 0.73 (corresponding to a mixture consisting entirely of non-compliant maize) and the maximum value is 4.26 (corresponding to a mixture consisting entirely of straw).

By analysing the values of the coefficients for Q and ash, one can observe that the best options are those for which the factors E (non-compliant wheat) and A (straw) are zero.

We obtain a graph that indicates possible values for factors B, C, D so that the calorific value and the residual ash fall between certain values (Figure 4.2). This figure indicates that it is possible to determine recipes for mixtures of 3 components for which the calorific value is greater than 18.5 MJ/kg, at the same time as the residual ash is less than 2% or recipes with a calorific value of 18.0 MJ/kg and residual ash below 2%. Less effective in terms of calorific value, but less desirable in terms of the amount of residual ash are also the cases Q> 17.5 MJ/kg and ash <1.5% and Q> 17.0 MJ/kg and ash <1.0%.

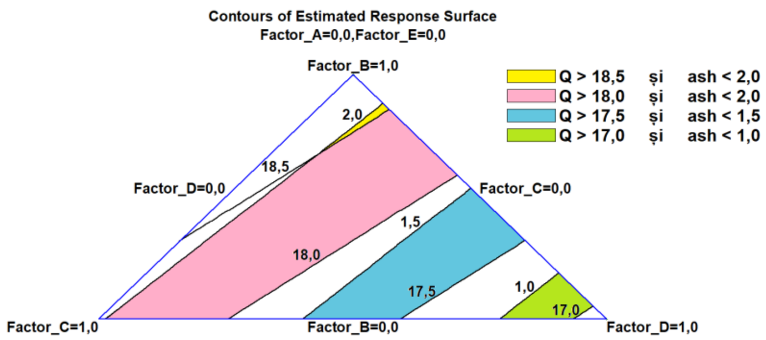

Figure 4.2 Possible values for calorific value and residual ash depending on the values of the experimental factors

4.3 Study of the influence of the additive on the quality of pellets obtained from a mixture of 2 types of biomasses

Experimental strategy

The aim of this experiment was to study the influence of the additive (in this case, corn grain) on the quality of pellets obtained from a mixture of two types of biomasses: fir sawdust and wheat grain.

Analysis of the influence of the composition on the calorific value of the pellets

The linear regression equation determined for the lower calorific value is

$$\begin{aligned} Q = {} & 9{,}95867 + 0{,}712252 \cdot \text{Grâu} - 0{,}503132 \cdot \text{Brad} - 0{,}159012 \cdot \text{Aditiv} - \\ & - 0{,}00638362 \cdot \text{Grâu}^2 - 0{,}0008125 \cdot \text{Grâu} \cdot \text{Brad} + 0{,}008875 \cdot \text{Grâu} \cdot \text{Aditiv} + \\ & + 0{,}00616284 \cdot \text{Brad}^2 - 0{,}00015 \cdot \text{Brad} \cdot \text{Aditiv} - 0{,}00296552 \cdot \text{Aditiv}^2 \end{aligned} \quad (4.3)$$

Imposing the condition $Wheat + Fir + Additive = 100\,(\%)$ and taking into account that the values for the percentage of wheat vary between 38% and 42%, and the additive - corn grains - is added in a percentage of maximum 5%, the diagram in Figure 4.3 is obtained.

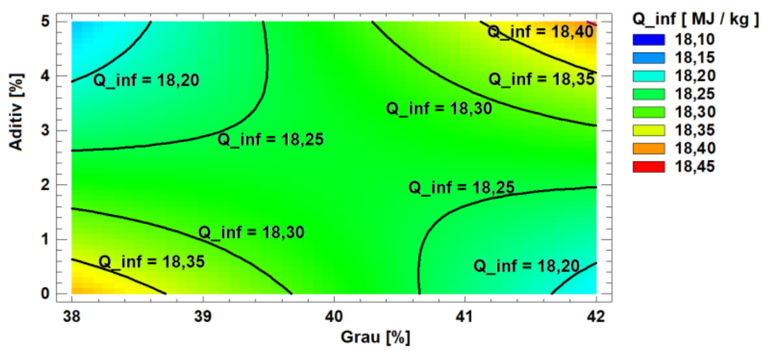

Figure 4.3 Level curves for Q_{inf}

Based on the formula deduced for Q, an extreme local point of the Q function can be calculated in the interval [38,42] × [58,62] × [0,5]. A minimum Q value of 18,262 MJ/kg is thus obtained for the recipe $Wheat: Fir: Additive = 40{,}068: 57{,}901: 2{,}031$. The maximum value for Q under these conditions is 18,404 MJ/kg, corresponding to the recipe $Wheat: Fir: Additive = 42: 53: 5$.

Similar results were obtained concerning the influence of the additive on the residual ash and the physical qualities of the pellets (length, diameter, bulk density, particle density).

4.4 Research directions and related activities

In addition to pellets and briquettes for heating, the company can diversify its business with minimal investment through:

- the inclusion in animal feed production
- inclusion in the production of fertilizers from sludge from sewage treatment plants
- use of willow bark for phytotherapeutic purposes

A solution to improve the quality of energy willow pellets involves peeling the wood. But this approach produces an industrial waste: bark. For sustainable development, willow bark should be used in one way or another.

Willow bark has been used as such or as an extract since ancient times for analgesic purposes. The active substance is salicin, which is contained in various percentages. In order to be used, dried willow bark must contain at least 1.5% salicylic derivatives, expressed as salicin content.

A methanol extract of willow bark provided by the partners from Rebina SA was analyzed in INCEMC laboratories, and the results of the chromatographic analysis show, qualitatively, the significant presence of a salicylic compound in the analyzed bark.

Thus, for *Salix alba*, after the separation of the bark, an increase in higher calorific value by 2,68% is obtained. On the other hand, at a production of willow of 7 tons/ha, 1169 kg of bark are obtained, which contain 16,0153 kg of salicin (at a percentage of 1,37% salicin in bark).

5 PROCESSING AND INTERPRETATION OF EXPERIMENTAL DATA USING OPERATIONAL RESEARCH TECHNIQUES

The objectives of this chapter are:

- To compile a database containing information on the raw material existing in the climate region specific to western Romania (elemental composition, calorific value, residual ash, price)
- To synthetise the current standards for the quality of heating pellets
- To establish a linear optimization model for pellet recipes
- To establish mathematical properties of the linear optimization model in the case of two-component mixtures, with or without additive
- To develop a preliminary software solution to determine an optimal mass ratio in the case of two-component mixtures without additive
- To develop a software solution that implements the linear optimization model for the built database and two-component mixtures, with or without additive
- To establish mathematical properties of the linear optimization model in the case of mixtures of $n \geq 2$ components, with or without additive
- To develop of a software solution that implements the linear optimization model for the built database and mixtures of $n \geq 2$ components, with or without additive

The original results are:

- a database with the properties of the various raw materials available for pelletizing
- an optimization problem (in 2 or more dimensions),
- mathematically necessary conditions for the solution of the optimization problem,
- algorithms for determining the solution of the optimization problem,

- software solution for determining the optimal recipe according to the user's options.

5.1 Databases used in the decision-making process

In order to make the decision-making process as efficient as possible, it is necessary to create the following databases: a database with applicable international standards in biomass production and a database with characteristics for the main types of biomasses that can be processed on the line technological.

The international standards applicable in the production of biomass for fuel are taken from ISO17225 and ENPlus and refer to the requirements on the origin of biomass, lower calorific value, ash concentration, and the concentration of noxious substances (N, S, Cl) in the combustion gases.

In order to implement the above-mentioned operational research results, a database was built with information on EU standards for pellets, the chemical composition of various types of biomasses and the price of raw material (in lei/kg). Where the information could not be determined by direct chemical analysis, the elementary chemical compositions of the raw material were taken from the literature ([11], [12], [14], [19]).

To determine the calorific value according to the elemental composition, Mendeleev's formula can be used which gives the calorific value in MJ/kg according to the percentage of C, H, O, S in the combustible material:

$$Q = 0{,}339 \cdot C + 1{,}029 \cdot H + 0{,}109 \cdot S - 0{,}109 \cdot O \qquad (5.1)$$

For a more precise result, applicable to the data in the database, we determined with the help of Statgraphics a regression equation for the calorific value, by which the calorific value is calculated (in MJ/kg) according to the percentage quantities of C, H, N , O, S, Cl of combustible material:

$$Q = 0{,}363504 \cdot C - 0{,}872841 \cdot Cl - 0{,}00671136 \cdot H + 0{,}316865 \cdot N + \\ + 0{,}0207733 \cdot O - 0{,}305485 \cdot S \qquad (5.2)$$

For this equation, the accuracy is 99.6018%.

5.2 Properties of the solution of the linear optimization problem in the case of a mixture of two components

Mathematically, for any two types of biomasses, 1 and 2, the standard linear programming problem is as follows:

$$\begin{cases} \max c = x_1 c_1 + x_2 c_2 \\ \text{dacă} \\ c_1 = 0.339\, C_1 + 1.029\, H_1 + 0.109\, S_1 - 0.109\, O_1 \\ c_2 = 0.339\, C_2 + 1.029\, H_2 + 0.109\, S_2 - 0.109\, O_2 \\ x_1 = \dfrac{m_1}{m_1 + m_2} \\ x_2 = \dfrac{m_2}{m_1 + m_2} \\ S = x_1 S_1 + x_2 S_2 \le S_{max} \\ N = x_1 N_1 + x_2 N_2 \le N_{max} \\ Cl = x_1 Cl_1 + x_2 Cl_2 \le Cl_{max} \\ ash = x_1 ash_1 + x_2 ash_2 \le ash_{max} \\ 0 \le m_1, m_2 \end{cases} \qquad (5.3)$$

where indices 1 and 2 refer to the two types of biomasses considered, C, H, S, O, N, Cl, refer to the mass concentration of the respective chemical element in the type of biomass considered, ash refers to the percentage of ash the type of biomass considered, and m_1 and m_2 are the masses with which the two raw materials contribute to the final mixture. The max index refers to the maximum value allowed for that component.

The main results regarding the properties of the linear programming problem are presented below.

Proposition 1 The necessary condition for the problem to have a solution is that

$$x_1 + x_2 = 1. \qquad (5.4)$$

We assume without restricting the generality that $c_1 > c_2$.

Proposition 2 If the problem has a solution, then

$$0 \leq x_1 \leq \min\left\{\frac{N_{max} - N_2}{N_1 - N_2}, \frac{S_{max} - S_2}{S_1 - S_2}, \frac{Cl_{max} - Cl_2}{Cl_1 - Cl_2}, \frac{ash_{max} - ash_2}{ash_1 - ash_2}\right\}. \qquad (5.5)$$

Proposition 3 The problem has a solution if and only if

$$\min\left\{\frac{N_{max} - N_2}{N_1 - N_2}, \frac{S_{max} - S_2}{S_1 - S_2}, \frac{Cl_{max} - Cl_2}{Cl_1 - Cl_2}, \frac{ash_{max} - ash_2}{ash_1 - ash_2}\right\} \geq 0. \qquad (5.6)$$

Particular cases Without restricting the generality, it is considered in the following only to the inequality corresponding to the concentration of N, for the other inequalities the reasoning and the results being similar. The sign of the ratio $R_N = \frac{N_{max}-N_2}{N_1-N_2}$ and the solution of the inequality $x_1N_1 + (1 - x_1)N_2 \leq N_{max}$ are studied. The following particular cases are distinguished:

1. $N_1 \leq N_2 < N_{max}$ Then the ratio R_N is negative and the problem has no solution.
2. $N_2 \leq N_1 \leq N_{max}$ Then the ratio R_N is positive, ant the problem could have solutions if all the other ratios involved are positive.
3. $N_1, N_2 \geq N_{max}$ The problem has no solutions.
4. $N_2 = N_{max}$ Then the inequation reduces to $x_1(N_1 - N_{max}) \leq 0$, which has solutions only if $N_1 \leq N_{max}$.
5. $N_1 = N_{max}$ Then the inequation reduces to $x_1(N_{max} - N_2) \leq N_{max} - N_2$, which has solutions only if $N_2 < N_{max}$.
6. $N_1 = N_2 \leq N_{max}$ Then the ratio R_N is positive, and the problem could have solution if all the other ratios involved are positive.
7. $N_2 \geq N_{max}$ Then the ratio R_N is positive only if $N_1 \leq N_2$. Moreover, because N_1 and N_2 cannot be simultaneously greater than N_{max}, it is necessary that $N_1 \leq N_{max}$.

Proposition 4 In the above-mentioned conditions, the maximum calorific value of a 2-component mixture is

$$c_{max} = c_2 + (c_1 - c_2) \cdot \min\left\{\frac{N_{max} - N_2}{N_1 - N_2}, \frac{S_{max} - S_2}{S_1 - S_2}, \frac{Cl_{max} - Cl_2}{Cl_1 - Cl_2}, \frac{ash_{max} - ash_2}{ash_1 - ash_2}\right\}. \qquad (5.7)$$

Taking into account the constraints stated above and by performing the substitution$x_2 = 1 - x_1$, the linear optimization problem becomes a problem of determining the maximum of a linear function of a single variable, which is reduced to the study of the monotony of the objective function.

Proposition 5 Let be the real constants $\alpha, \beta, \gamma, \delta$ and the problem of determining the maximum of a linear function of a single variable

$$\max_{\gamma \leq x_1 \leq \delta} (\alpha x_1 + \beta) \qquad (5.8)$$

Then the following statements are true:

a. If $\gamma > \delta$ then the problem has no solutions.

b. If $\gamma = \delta$ then the problem has a unique admissible solution, $x_1 = \gamma$, which corresponds to $x_2 = 1 - \gamma$. This solution is optimal and the value of the objective function is $c = \alpha x_1 + \beta$.

c. If $\gamma < \delta$, then the problem has the following solutions, depending on the parameter α:

i. If $\alpha > 0$ (the case in which the objective function is strictly increasing), the optimal value is obtained for $x_1 = \delta$ (which corresponds to $x_2 = 1 - \delta$) and is $c = \alpha\delta + \beta$.

ii. If $\alpha < 0$ (the case in which the objective function is strictly decreasing), the optimal value is obtained for $x_1 = \gamma$ (corresponding to $x_2 = 1 - \gamma$) and is $c = \alpha\gamma + \beta$.

iii. If $\alpha = 0$ (if the objective function is constant), there exist an infinity of optimal solutions, corresponding to $x_1 \in [\gamma, \delta]$, and the optimal value is $c = \beta$.

Based on Proposition 5, a simplex algorithm was built to determine the calorific value of two-component mixtures [15].

A particular case is the case where the mixture contains additives, thus in addition to component x_1 and component x_2 there appears also a component x_a. However, knowing the nature of the additive (elemental chemical composition, calorific value and ash) as well as the amount of additive added, new maximum standard values for N, S, Cl and ash can be calculated. With these maximum values, the optimization problem is reduced to the problem of determining a recipe without additives.

The algorithm for determining the calorific value allows the calculation of both an optimal recipe without additives and one with additives. It is implemented in C and has an interface that allows it to be easily used by users. The program allows several options: consulting international standards, determining an optimal recipe based on data in an adjacent file, adding new material to the adjacent file.

The adjacent file, which contains the raw materials, is structured in lines, each line being of the type

material	C	H	O	N	S	Cl	Price	Q_inf	ash

Option 1, consult the standards, has the effect of displaying the limitations (on N_{max}, S_{max}, Cl_{max}, ash_{max}, $additive_{max}$) imposed by the 8 predefined standards:

For option 2, determine a recipe, the file containing the database is browsed, and the user must choose the name of the materials that could be part of the new recipe. Then, the user can choose one of the predefined standards or can impose his own maximum values that will be considered for N, S, Cl, ash, additive.

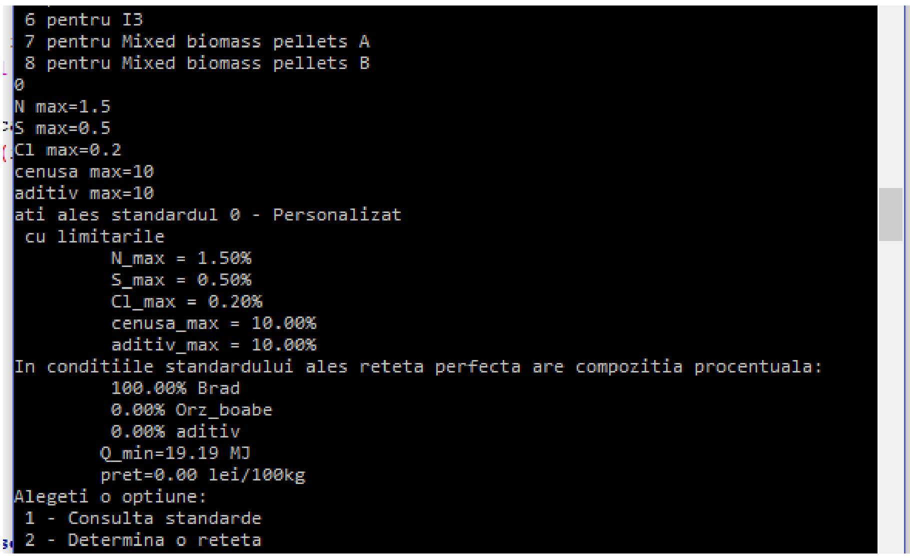

Figure 5.1 Using a custom standard in a recipe

If an additive is to be added to the composition, the calculations are made for the maximum permissible value of this additive. The choice of an additive also influences the limitations imposed by the standards, and the new values are displayed. If a custom standard is desired, it can be entered by the user.

The answer of the program is presented below for a recipe based on fir and barley grains was chosen, without additive and with maximum allowed values of 1.5% for N, 0.5% for S, 0.2% for Cl, 10% for ash and 10% for additive.

If it is desired to add a new material to the database, the user is warned that it is imperative to know the percentage values for N, S, Cl, ash and calorific value Q in MJ/kg.

5.3 Linear optimization problem for n-component mixtures, $n \geq 2$

Given n raw materials for which the elementary concentrations C, H, S, O, N, Cl, the ash concentration and the calorific value are known (in MJ/kg), the problem is to determine the composition of that mixture for which the concentrations of N, S , Cl and ash remain below certain limits and in addition the calorific value of the mixture is maximum.

If $n > 2$, the solution of the problem cannot be determined immediately. Instead, the existence of the solution and, if so, the mass value of the n components of the mixture can be determined using the simplex algorithm, similar to the case $n = 2$.

5.4 The application for determining optimal pellet recipes from the perspective of the possibility of a technology transfer

The basic principles, the technological concept, its functionalities and characteristics have been demonstrated at analytical or experimental level. The components were validated in laboratory conditions (TRL4), then in the industrial environment, at the factory in Cenei, starting with 2018.

The prototype is being validated on a full scale (TRL6) in a factory specializing in the production of pellets and briquettes for heating.

The maturity phase of the technology proposed in this research (i.e., the functionality of the product under relevant operating conditions (TRL 7), the completed and qualified system (TRL 8) and the demonstration in operational environments of the product functionality (TRL 9)) is to be reached in -a near future.

6 PROCESS VALIDATION, OPTIMIZATION AND PREDICTION USING ARTIFICIAL INTELLIGENCE ELEMENTS

The objectives of this chapters are:

- To build an artificial neural network to determine the elementary composition of a solid fuel, if its calorific value and the residual ash resulting from its combustion are known.
- To use the network outputs to determine the calorific value, using a specially determined regression formula.
- To compare the results obtained with the experimental data and to determine the conditions under which the theoretical solution (neural network + regression) can be applied in practice.

The original results obtained in this chapter are:

- a neural network for determining the elemental composition of a material, starting from its calorific value and the residual ash resulting from combustion
- an assessment of the possibility of applying this method in combination with the software solution detailed in the previous chapter to determine optimal pellet production recipes

6.1 Building of a neural network to determine the basic composition of fuels

In order to build a neural network, first it is necessary to state a number of general considerations related to process parameters and working technique, and then to detail the architecture of the neural network that will be built.

The calculations were performed using the Neural Networks toolbox from Matlab [7].

The input data set was randomly divided into the test set (71,06% of entries, i.e., 54 entries), the validation set (14,47% of entries, i.e., 11 entries), and the test set (14,47% of entries, i.e., 11 entries). Each entry is of type

Q_inf	ash

and each output of the type

C	H	O	N	S	Cl

Therefore, the neural network is a function

$$\mathbf{y} = f(\mathbf{x}) \qquad (6.1)$$

where $\boldsymbol{y}$ is a 6-element vector corresponding to the percentage elementary chemical composition (C, H, O, N, S, Cl), and $\boldsymbol{x}$ is a 2-element vector, corresponding to the values for the lower calorific value in MJ/kg and the amount of ash into the %.

The neural network has an input layer with 2 neurons, two hidden layers with 10 and 6 neurons, respectively, and an output layer with 6 neurons (Figure 6.1).

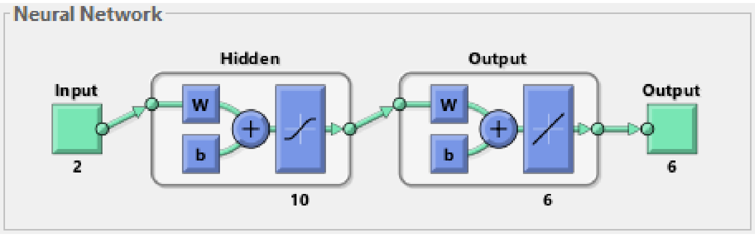

Figure 6.1 ANN structure that binds the elemental composition to the calorific value and residual ash of a material

Two networks were created: a network trained by the Levenberg-Marquardt algorithm (implemented with the Matlab trainlm function) and one trained by the Bayesian regularization (implemented with the Matlab trainbr function).

In both cases, the network training algorithm involves the following steps:

Initialization of weights with random values

Repeat training epoch:

    For each input data set:

        Performs the forward step, applying the transfer function to the neurons on the input layer

        Perform the backward step

        Adjust weights

    Recalculates the error function

Until the stop condition is met

The Levenberg-Marquardt algorithm uses both the training set and the validation and testing set for network construction. The accuracy of the network for the training stage is 0,99667, for the validation stage it is 0,9968, and for testing it is 0,99042. In total, the built-in network has an accuracy of 0,99581.

The Bayesian regularization algorithm uses only the training set and the test set. The validation itself is included in the algorithm. The accuracy of the network for the training stage is 0,99875, and for the testing stage it is 0,99235. Overall, the accuracy of the network is 0,99784.

6.2 Usage of the designed network architectures to predict the physical properties of different mixtures

The two neural networks created in the previous paragraph were used to determine the elementary composition of the components. Then, based on the values returned by the two neural networks, the calorific value was reconstituted and compared with the experimentally determined one. Calorific value was calculated in two ways:

a. using Mendeleev's formula

b. using the regression equation that we determined in Chapter 5, paragraph 5.1, using Statgraphics and for which the accuracy is 99,6018%:

While the accuracy of the network built with the Levenberg-Marquardt algorithm is good, 99,581%, the data returned by the network have no correspondent in practice. Thus, for a number of 9 recipes out of the 15 for which we tested the algorithm, the Cl value has negative values - which is physically impossible.

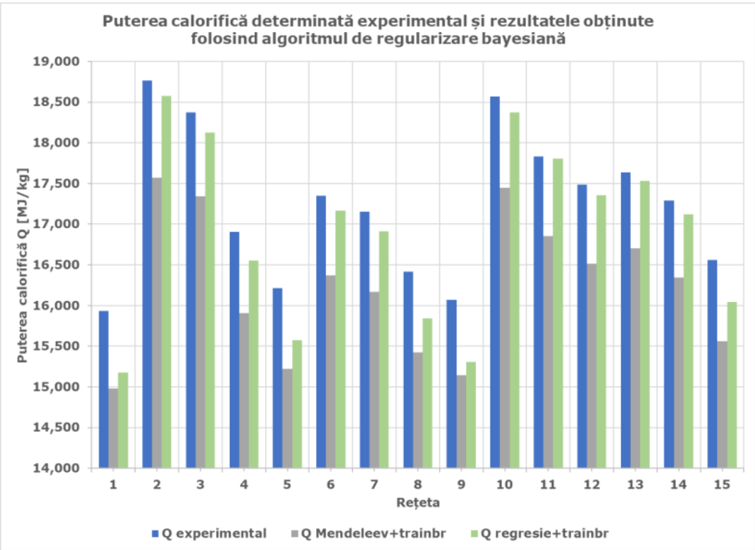

Figure 6.2 Comparison between experimental and calculated results with the Bayesian regularization algorithm

The network built using Bayesian regularization poses no practical problems, at least not for the experimental data set used for testing. In addition, the accuracy of this network (99,784%) is higher than the accuracy of the network trained by the Levenberg-Marquardt algorithm. Therefore, the use of the network trained with the Bayesian regularization algorithm is preferable.

For the data provided by both algorithms, the formulas for determining the estimated calorific value were applied. By applying Mendeleev's formula to the outputs of neural networks, both in the case of the trainlm function and in the case of the trainbr function, the values for the calorific value are lower than the experimental values. Moreover, in general, the values corresponding to the trainbr-trained network are generally lower than those corresponding to the trainlm-trained network.

Therefore, using the combination of the trainbr-trained network and the regression determined on the basis of the network outputs, the results are closer to the experimental results - hence the error is smaller.

7 GENERAL CONCLUSIONS. PERSONAL CONTRIBUTIONS. PERSPECTIVES OF RESEARCH

7.1 General conclusions

Based on the need for innovation in the production of pellets and briquettes for heating, expressed by a company operating in the field, the present research provided a series of answers related to the innovation of the production line, the possibility of diversifying production and determining optimal recipes given the raw materials available for processing.

The contributions brought to light by the thesis will be presented below.

7.2 Personal contributions

Personal contributions are theoretical, experimental or industrially applicable, are based on documentary studies, theoretical modelling and experimental research conducted during the doctoral stage. These will be summarized below, together with their importance and areas of applicability.

Theoretical contributions

- **building a database with the biomass that can be processed in the area.** This result contributes to the achievement of the primary objective OP1 and the achievement of the secondary objectives OS3 and OS4.
- **construction of a neural network that predicts the elementary composition of a material based on its calorific value and the amount of residual ash of this material.** This result contributes to the achievement of the primary objective OP1 and the secondary objectives OS3 and OS4.
- **determination of a model for the calorific value and residual ash of the pellets based on the composition of the recipe from which they were produced.** This result contributes to the achievement of the primary objectives OP1 and OP2, but also the secondary objectives OS3 and OS4.
- **writing the problem of linear optimization associated with the production of pellets for heating in the case of mixtures of two or more components.** This result contributes to the achievement of the primary objectives OP1 and OP2 and the secondary objectives OS2, OS3, OS4.
- **determination of mathematical properties of the linear optimization problem in the case of two-component mixtures and in the case of multi-component mixtures.** This result contributes to the achievement of the primary objectives OP1 and OP2 and the secondary objectives OS2, OS3, OS4.

Experimental contributions

- **factory verification of the feasibility of various types of pellets whose recipes were theoretically obtained.** This result contributes to the achievement of the primary objective OP1 and the secondary objective OS1.
- **checking the properties of empirical mixtures of pellets.** This result contributes to the achievement of the primary objective OP1 and the secondary objectives OS1, OS3.
- **checking the influence of the additive on the quality of the pellets.** This result contributes to the achievement of the primary objective OP1 and the secondary objectives OS1, OS3.

Industrially applicable contributions

- **premises for optimizing the technological line by attracting European funds.** This result contributes to the achievement of the primary objectives OP1 and OP2 and the secondary objectives OS2, OS3.
- **possibility of optimizing the pellet recipes for heating using the software solutions developed.** This result contributes to the achievement of the primary objectives OP1 and OP2 and the secondary objectives OS3, OS4.
- **premises for the production of animal feed.** This result contributes to the achievement of the primary objective OP2 and the secondary objective OS3.
- **premises for the production of agricultural fertilizers.** This result contributes to the achievement of the primary objective OP2 and the secondary objective OS3.
- **premises for improving the quality of willow pellets and the sustainable development of the company by capitalizing on willow bark for phytotherapeutic purposes.** This result contributes to the achievement of the primary objective OP2 and the secondary objective OS3.

7.3 Prospects for further development

Following the experience gained during the doctoral research internship, the following directions of further development were identified:

- further improvement of the production line by adding new equipment and automation techniques
- the possibility of producing fodder that meets the nutritional requirements of certain categories of animals or the production of a "universal" fodder that meets the nutritional requirements of as many categories of animals as possible
- the possibility of using sludge from sewage treatment plants for the production of fertilizers, while developing a database with them to advise farmers on their safe and legal use
- separation of willow bark in order to improve the quality of pellets for heating, while determining optimized recipes for pellet mixtures and capitalizing the bark for phytotherapeutic purposes
- offering optimal, customized solutions, starting from databases and models built in the areas mentioned above
- transforming the software solution developed in the thesis into a more user-friendly one and achieve a wider use in the production of pellets and briquettes for heating

This paper contains both theoretical and experimental and industrially applicable results that can become a transfer of technology from the academic and industrial research environment to the business environment. The results are the basis of 9 scientific papers, of which 7 are indexed in Web of Science and 2 are indexed in other international databases. It is the premise of increasing competitiveness for both companies in various fields that make pellets.

The current level of technological readiness of the software solution proposed in the thesis is TRL 6 - being currently tested on a real scale in a pellet company from Cenei. In the future, the results of the research will be implemented in functional environments on a larger scale, thus reaching all stages of development of a technology transfer project.

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