ARTIFICIAL NEURAL NETWORKS FOR PREDICTING THE GENERATION OF ACETALDEHYDE IN PET RESIN IN THE PROCESS OF INJECTION OF PLASTIC PACKAGES

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Abstract

The industrial production of preforms for the manufacture of PET bottles, during the plastic injection process, is essential to regulate the drying temperature of the PET resin, to control the generation of Acetaldehyde (ACH), which alters the flavor of carbonated or non-carbonated drinks, giving the drink a citrus flavor and putting in doubt the quality of packaged products. In this work, an Artificial Neural Network (ANN) of the Backpropagation type (Cascadeforwardnet) is specified to support the decision-making process in controlling the ideal drying temperature of the PET resin, allowing specialists to make the necessary temperature regulation decisions for the best performance by decreasing ACH levels. The materials and methods were applied according to the manufacturer's characteristics on the moisture in the PET resin grain, which may contain between 50 ppm and 100 ppm of ACH. Data were collected for the method analysis, according to temperatures and residence times used in the blow injection process in the manufacture of the bottle preform, the generation of ACH from the PET bottle after solid post-condensation stage reached residual ACH levels below (3-4) ppm, according to the desired specification, reaching levels below 1 ppm. The results found through the Computational Intelligence (IC) techniques applied by the ANNs, where they allowed the prediction of the ACH levels generated in the plastic injection process of the bottle packaging preform, allowing an effective management of the parameters of production, assisting in strategic decision making regarding the use of temperature control during the drying process of PET resin.

Keywords: Drying Temperature, Artificial Neural Networks, Computational Intelligence, PET, Acetaldehyde.

1. Introduction

The population increase and technological advances, have been providing an improvement in the quality of life and convenience for the population. Enabling research and development of new technologies and raw materials for the generation of new products.

Polyethylene terephthalate (commonly abbreviated as PET, PETE or by resin identification) (recycling code # 1) is one of the most diffuse thermoplastic polymers available on the market [1].

The advantages of PET in relation to glass, such as weight and practicality, have made the use of PETs in products increasingly greater. A PET bottle, for example, is much lighter than a glass one, making it a safe and easy to transport container.

In this context, processes that increase the efficiency of the manufacture of plastic products have shown a considerable increase [2].

PET, thermoplastic polyester, is widely used in industrial applications such as packaging, beverage bottles, power tools, sporting goods and textile fibers. It has good mechanical, physical, and properties barrier chemical and gas [3]. It presents advantages and properties, such as: Cheap cost, Light Packaging, High Mechanical and Chemical Resistance, Versatility in formats and colors, High Barriers to Gases, excellent transparency and brightness [4].

PET is chemically classified as a thermoplastic polyester polymer with a partially aliphatic and aromatic semicrystalline structure, and is one of the most important of the polyesters [5]. It is the ideal Thermoplastic for many applications, mainly in the packaging segment, and especially in carbonated beverage bottles.

The choice of packaging material is essential to preserve the food characteristics: in particular, the adoption of polyethylene terephthalate for drinks helps to seek the quality and safety of the food due to its own characteristics, as a barrier to gases and aromas, transparency and easy processing [6].

The polymer is mainly used for the production of bottles/containers for beverages, such as water (ca. 26%), carbonated soft drinks (soft drinks, about 26%) or other drinks/juices (about 18%), in the form of sheets/films (ca. 14%), in the food industry (ca. 9%), as well as in non-food uses (for example, cosmetics, ca. 6%)[1].

First of all, PET is a thermoplastic polymer, which means that it can be easily processed again at a high temperature. In addition, PET can be easily recycled, as almost all bottle production. The beverage industry (ie water and soft drinks) uses this specific polymer extensively (as previously discussed). In particular, the PET recycling industry is very efficient and PET processing allows different scenarios to be obtained [1].

In world production, plastic packaging and containers have the greatest application (36%) among industries, applications of world production of plastics (approximately 400 million per year), followed by construction materials (16%) and textiles (14%). Global plastics production is expected to increase continuously from 300 million tons in 2015 to 1800 million tons in 2050 [7].

In 2016, the production of packaging was of the order of 17.5 million tons, reaching an increase of 4.8%. This growth was due to the development of new products for application in several areas of the canning, juices and other functional drinks industry, prediction in the drop in PET resin prices will stimulate the consumer market. [2].

Plastic beverage containers are mainly formed by the Injection Stretch Blow Molding (ISBM) process. ISBM is the common choice for manufacturers of plastic containers for the manufacture of beverage packaging [8].

PET is the most widely accepted material for manufacturing of plastic molds due to its mechanical and resistance properties. In the injection blow molding process, the parison (or pre-mold) is injection molded on a steel rod, then the molded preform is transferred to the next station where the application of the elongation through an elastic rod and the application of a pressure causes the preform to expand inside the mold. [8].

During the injection molding process, which essentially consists of heating and softening the material grains in a heated cylinder and its consequent injection at high pressure into the mold, where it cools and takes its final shape. [9].

The complete injection process for obtaining injected parts is divided into five stages: drying (silo), feeding, plasticizing, injection and extraction of the parts [9] [10].

Polyethylene terephthalate is a hygroscopic material: it absorbs water from the environment. During its storage (ensilage), rigorous and controlled drying in PET resins is essential before its transformation. To obtain the required levels of drying, peripherals such as silo (ensilage), dryers with desiccants (usually with molecular sieves) are necessary, where the air used for drying the resin is previously dehumidified, polymers and PET do not escape the rule, where the interval of recommended drying temperature, which should be between 4 to 6 hours otherwise, excessive temperatures can occur and can damage the raw material, the temperature of the dry air used for drying must be between 160ºC - 180ºC (measured at the dryer outlet) when the air temperature dry should not exceed 190ºC [9].

A problem that arose and the formation of Acetaldehyde (ACH), during the polymerization of PET resin [11].

The high temperature of heat treatment during the synthesis of PET results in the formation of final carboxylic groups and vinyl esters. The combination of these groups generates vinyl alcohols as a by-product, which may exist in its tautomeric form, that is, as acetaldehyde. The organoleptic detection limit for acetaldehyde is very low, ranging from 4 to 65 µg.kg [12].

The formation of Acetaldehyde is aggravated when the PET polymer is exposed to high temperatures, normally used during the plastic injection process. When the polymer is heated above the melting temperature, it can generate high levels of ACH that can alter the flavor of the carbonated and non-carbonated drink [13].

By controlling the critical stages of the injection process in the production of PET bottles, it is possible to keep the formation of acetaldehyde at low levels.

To obtain a bottle with a low content of ACH within the specifications required by the quality control, during the transformation of the PET resin: low temperature of the molten resin, low shear rate and low residence time [4].

The Artificial Intelligence techniques applied to the field of the plastic injection process aim to assist in the decision process of selecting values for the process parameters deduced from a qualitative inspection of injection defects. The objective of such systems is to optimize the process conditions to obtain a part with the specified quality [14].

AI in injection molding machines can make an important contribution in the production of quality plastic parts, due to the action of sensors that monitor variations in the temperature of the grains, subjected to factors that may disqualify the results obtained in the injection [15].

Systems based on Artificial Intelligence (AI) are being applied in the most diverse areas of the industry. The implementation of systems for operations in the injection molding process suggests optimal conditions for the management of AI-based parameters, which represent a great level of reliability in the process conditions. The main objective of this work is the specification of an Artificial Neural Network (ANN) to control and predict the formation of acetaldehyde in the plastic injection process of the preform for PET packaging production.

2. Literature review

2.1. Injection molding

Simultaneous processes injection molding, also classified as injection processes with more than one component, demonstrate a great potential in the finishing of injected parts, precisely because they allow the finishing application to be carried out during the injection process, as well as by the greater flexibility possible variations in finishes that can be used [16].

These processes have been widely used in several segments of the industry, from simple components, such as toys and pots, to complex structures that will be subjected to high levels of vibration and load [17].

Injection molding is one of the most used methods in the manufacturing of polymeric products, due to its flexibility and high degree of manufacturability. In this process, the melted polymer is injected into a mold cavity with a desired shape and then cooled under high pressure [18].

In this cooling phase, when the part becomes rigid enough to be extracted from the mold, extra care is necessary, as this phase directly and mainly affects the productivity and quality of the molding. [19].

The plastic injection molding process is a process that can be controlled by predefined parameters. The injection mold can be manufactured with a single cavity or in *n* similar or dissimilar cavities. The cavities are interconnected through flow channels or corridors that direct the flow of the molten plastic material into the cavities.

The plastic injection molding cycle consists of four phases: plasticization, injection, packaging and cooling. Therefore, several process parameters, which include melting temperature, mold temperature, injection pressure, injection speed, injection time, packaging pressure, packaging time, cooling temperature and cooling time, all potentially influence the quality of injection molded plastic products [20].

The quality characteristics of plastic injection molded products can be categorized according to dimensional properties, surface properties and mechanical properties. Inadequate settings of the process parameters can cause many defects in the product, which are classified as surface properties and defects of mechanical properties. Thus, the appropriate configurations of production conditions can shorten the production cycle and improve the quality of plastic injection molded products. [20].

The injection cycle of the preform is carried out as follows: Closing the mold; Advance of the injection unit; Injection; Repression; Recoil (machine cannon); Dosage; Opening the mold and extracting the part.

2.2. PET packaging production

For the manufacturing of a higher molecular weight polymer, resins for bottle production, the amorphous grains are subjected to an additional stage of solid state polymerization until reaching a degree of polymerization equal to 160 and an average molecular weight of 60,000. The average molecular weight of the polymer increases as ethylene glycol is released and removed and acetaldehyde levels reduced to concentrations below 3 mg/kg [21].

The resin is ready to be used in the production of preforms, which will later be transformed into PET bottles. For the injection of the preform, the resin is heated to temperatures of 270° C, injected into the mold cavities and cooled very quickly in order to maintain the molecular structure predominantly in amorphous form, thus avoiding recrystallization. The preform is heated to 90-100° C and then blown to produce the bottle [21].

2.3. Molding Machines

Plastic injection molding machines meet different qualitative specifications to produce specific parts such as dry cycle, injection rate and injection pressure [22]. The types of injection molding machines can be characterized by their three most common methods of operation which are: hydraulic, electric and hybrid. Two systems basics plasticization are observed, the first being the single-stage molding system (Figure 1) and the second, two-stage molding system (Figure 2). There are also three-stage molding units, etc. The double stage is the piggyback, which can partially be related to a continuous extruder [22].

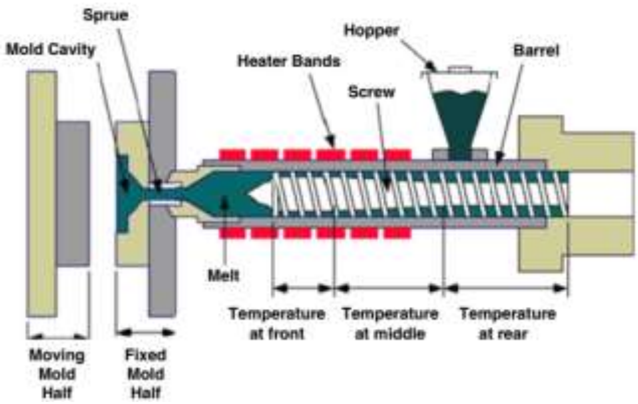


Figure 1. Simple plasticizer cannon for injection molding machines.
Source: [23]

The simple stage shown in figure 1, is known as the alternate screw of the injection molding machine.

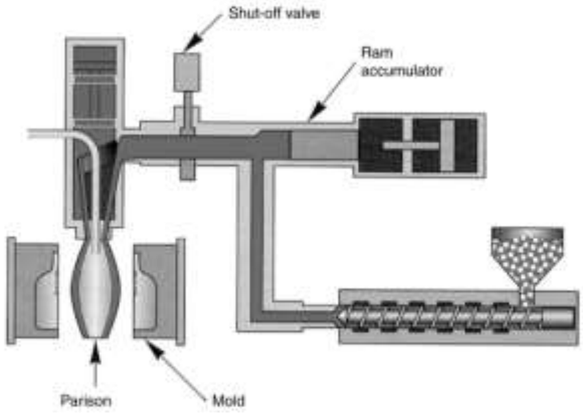


Figure 2. Double plasticizer cannon for injection molding machines.
Source: [24].

Drying the PET polymer is one of the most important processes of this step. In the solid state, the PET polymer, being hygroscopic, absorbs moisture up to the equilibrium value with the relative humidity of the local environment and in environments of high relative humidity it can reach up to 0.6% (w/w) by weight, if it is exposed without no protection and long-term weather. In practice, if the polymer is stored in closed places, properly packaged and for short periods of time, the moisture value is lower and may be less than 0.1% (w / w) of the weight, before the polymer melts, due to hydrolyzation, reducing the molecular weight and, consequently, the physical, chemical and physicochemical properties [13].
Subjecting the resin to fusion with these moisture levels, will result in rapid degradation (hydrolysis), reducing its molecular weight (Figure 3), which is reflected in the loss of intrinsic viscosity and consequent loss of its physical properties. To maintain the maximum performance of PET polymers, its moisture content must be reduced to levels below 0.003% (30 ppm). [9]
Careful and controlled drying of PET resins is an essential operation before their transformation.

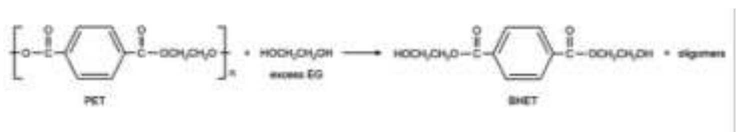


Figure 3. Reaction of hydrolytic degradation (hydrolysis) of PET resins.
Source: [25].

2.4. Acetaldehyde

The Acetaldehyde (ACH) is a clear liquid that burns easily. It has a strong, fruity odor that can make breathing difficult in high concentrations. Acetaldehyde is also referred to as ethanal and forms naturally in the body and in plants [26]. In the food industry, many odorous compounds are produced during the fermentation process of yeast and in processes without control systems, a large amount of odorous compounds are released into the atmosphere. In food fermentation, mostly volatile organic compounds such as ethanol and acetaldehyde are released and cause odor problems [26].

ACH is miscible in water and in various solvents, and in diluted concentrations it presents the aroma of citrus fruit. The most common synonyms for Acetaldehyde are ethanol, acetic aldehyde, acetylaldehyde, ethylaldehyde, diethylacetal and 1,1 - diethyloxyethane, whose molecular structure is shown in Figure 4, [27].

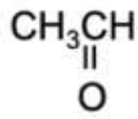


Figure 4. Acetaldehyde structural formula.
Source: [28]

2.4.1 Generation of Acetaldehyde in the manufacture of resin PET

During synthesis/processing of PET at temperatures above the melting point (ca. 260 ◦C), it is possible to form chain scission involving terminal ends with consequent release of undesired acetaldehyde [1].

The use of PET in the bottled water/drinks sector presents some drawbacks that should be faced too. In particular, the high sensitivity of PET esters bonds against water molecules as well as all its possible degradation products (one above all the release of acetaldehyde) still remain critical issues that deserve attention by experts, especially considering the high use of this polymer in the packaging industry for food contact [29].

ACH is formed during the polymerization phase, in the manufacture of PET resin. The amorphous grain obtained at this point can contain between 50 ppm and 100 ppm ACH, depending on the temperatures and residence times used in the process. The resin is post-condensed in a solid state, until it reaches the ideal molecular weight for the manufacturing of bottles. During this stage, the ACH diffuses out of the grain together with the glycol, being carried by the process's N2. Thus, the ACH of the PET in the bottle that leaves the solid post-condensation stage reaches residual ACH levels lower than (3 or 4) ppm, according to the specifications required by beverage manufacturers, and may reach levels below 1 *ppm* [9].

In particular, the high sensitivity of PET esters bonds against water molecules as well as all its possible degradation products (one above all the release of acetaldehyde) still remain critical issues that deserve attention by experts, especially considering the high use of this polymer in the packaging industry for food contact [1].

2.5. Generation of Acetaldehyde in the molding process

In the resin molding process (PET), the melting temperature is a key variable to control the generation of the formation of acetaldehyde (ACH), it is in this process that essentially consists of softening the material in a heated cylinder [22].

It is possible to obtain low residual levels of ACH, in the production of PET resin for packaging. This residual is generated during the melting of the polymer in the injection molding phase of the preform. Becoming important to control the injection process in which the polymer is exposed to high melting temperatures for a prolonged time [30].

In addition to the prolonged time at the melting temperature, other relevant factors that are responsible for the levels of acetaldehyde found in PET packaging, such as type and formulation of the resin, type of equipment, drawing of the screw thread profile of the cannon of injection machine, must be considered and transformation conditions [11].

The manufacture of PET bottles obtained by the per blowing injection process, makes it possible to obtain the following characteristics, ideal for the Carbonated Soft Drinks segment (CSD) [1]:

- PET is colorless and can be transparent (if amorphous) or translucent (if semi-crystalline). This is a very important characteristic as it allows consumers seeing the content within the bottles.
- PET is lightweight. The weight of a 1L PET bottle designed for containing water is ca. 25 g. For comparison, a 750 mL wine bottle made by glass is ca. 360 g weight, and a 500 mL aluminium can typically used for CSD is ca. 18 g weight.
- PET is thermoplastics, robust, semi-rigid to rigid, mechanically resistant to impact, and stretchable during processing.
- PET shows gas-barrier properties against moisture and CO2 (this is important for CSD).
- PET is extremely inert compared to the other plastics, and free from plasticizers (on the contrary, in the case of PVC the use of plasticizers is essential).

The flavors and aromas of drinks in general can be altered by the presence of (ACH), which may come from the environment, the product itself and/or the packaging material used [9].

The concern with the presence of Acetaldehyde in PET packaging is due to the possibility of altering the taste of the final packaged product. Soft drinks and mineral water are products in which the flavor is directly affected by the presence of ACH. Mineral water without gas are more sensitive, resulting in a low level of taste perception, in the range of 20 ppm to 40 ppm ACH, depending on the composition of the water [30]. During synthesis/processing of PET at temperatures above the melting point (ca. 260 ◦C), it is possible to form chain scission involving terminal ends with consequent release of undesired acetaldehyde [1].

PET is a polyester belonging to the group of condensation polymers. Polymerization takes place in two stages. In the first stage, esterification occurs of the diacid or diester with ethylene glycol producing the monomeric diester, bis (2-hydroxyethyl) terephthalate (BHET), as shown in Figure 5, [21].

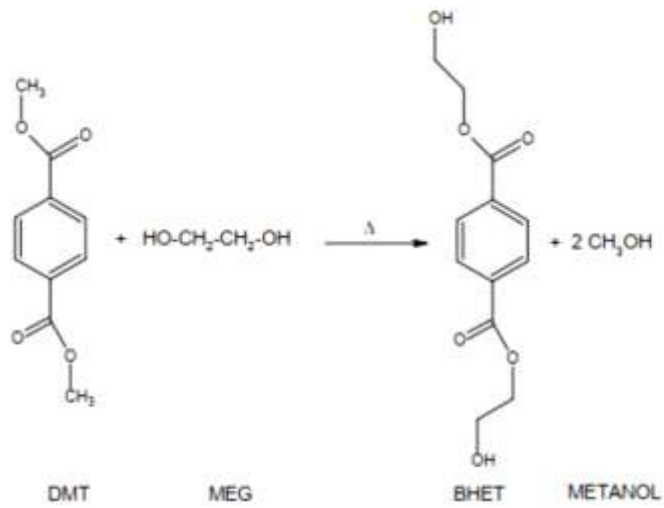
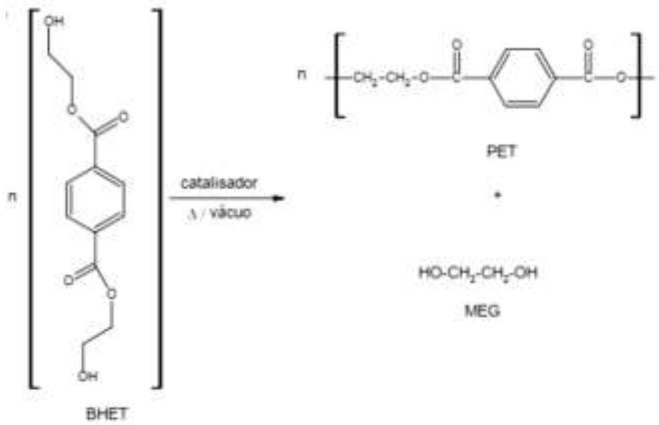


Figura 5. Polimerização de PET. Reação de conquista monômero BHET.

Source: Adapted of the [21].

When the starting substance used is terephthalic acid (PTA) the reaction is known as direct esterification reaction and when dimethyltereftalate (DMT) is used the reaction is known as transesterification reaction [21].

In the second stage, BHET continues to condense (polycondensation reaction) increasing the molecular weight until the polymer is formed (Figure 6). During this process, ethylene glycol (MEG) molecules are released and recycled for reuse. PET in its molten state is subjected to extrusion, and *pellets* are then formed



[21].

Figure 6. BHET polymerization to obtain PET resin.

Source: Adapted of the [21].

PET is sensitive to thermal degradation, especially in the presence of water and / or oxygen. A common product of thermal degradation of PET is the ACH [21].

ACH measurements made in the various stages of the injection-blow process, in bottle preforms, confirm that the main source of ACH generation in the PET resin transformation process occurs during the injection of the preform, due to the reflow of the resin [9].

The ACH generated during the PET blow-injection is retained on the bottle wall between the polymer molecules, slowly diffusing to the contents of the bottle. [30]

Control of the generation of ACH in the manufacture of bottles, the ACH formed in the bottle depends on: [9].

- Formulation of the resin;
- Transformation conditions.

At high temperatures, significant levels of ACH are generated. Thus, the control of the injection process is essential to control the generation of ACH in the production of bottles. On the other hand, the blowing step has practically no effect on the formation of ACH, since it works at milder temperatures.

Thus, to reduce the generation of ACH from the resin during injection of the preform, it is advisable to keep the melted polymer at the lowest possible temperature for the minimum time, with a minimum of shear.

The concentration of ACH in the preform increases in the same proportion as the drying temperature, of the cannon and that of the mold. But just adjusting the temperatures of the cannon and the mold channels does not guarantee that the temperature of the molten polyester will remain adequate. The viscous molten polymer is also heated by friction with the cannon, the thread and the distribution channels. This friction is a function of both the viscosity of the molten resin and the type and rotation of the thread. In addition to the heat generated by friction, the shear breaks mechanically like polymer molecules, thus forming more bis (2-hydroxyethyl) terminal groups, which in turn form more ACH (Figure 5) [9].

The parameters to be controlled to minimize exposure to heat are:

a) Cannon temperature (decrease);
b) Temperatures of the hot runner, manifold and nozzles (decrease);
c) Residence time in the cannon, manifold and in the hot runner (keep as little as possible);
d) Residence time of the melted polymer in the process.

A parameter of almost equal importance to the temperature of the molten polymer, to minimize the formation of ACH in the preform, is its residence time. Simply put, it is noted that the generated ACH is almost directly proportional to the residence time of the polymer melted in the process. Thus, it is a good norm to minimize cycle time to decrease the generation of ACH.

Parameters that depend on the machine used:

- Dimensions of injection channels;
- Of the screw thread profile.

Since low concentrations of ACH already affect the organoleptic properties of mineral waters and cola-type soft drinks, the manufacture of bottles with low ACH is essential for the rigid packaging industry. Therefore, the analysis of ACH in the quality control of resins and bottles is preponderant. [30].

2.6. Artificial Neural Network

Artificial Neural Network (ANN) is inspired from human neural system and it is used in different areas like pattern recognition, optimization, control and etc. Neural network is composed of several processing units (nodes) and directed links between them. These connections are weighted representing relation between input and output neurons [31].

An ANN is a set of artificially structured neurons that are trained from a specific sequence of steps (algorithm) to obtain the desired output. The main design of ANNs is adapted from the fundamental structure of a biological neuron that resides in our brains [32].

2.6.1 Perceptron

A mathematical perceptron of a biological neuron was proposed almost 65 years ago by McCulloch and Pitts in 1943 to replicate the functioning of a biological neuron [32].

Even though research in neural modeling started circa 1940 (i.e., McCulloch & Pitts in 1943), there was little active development of the field prior to the late fifties and early sixties when Rosenblatt introduced the perceptron in 1958, in figure 7 the basic structure of a perceptron [33].

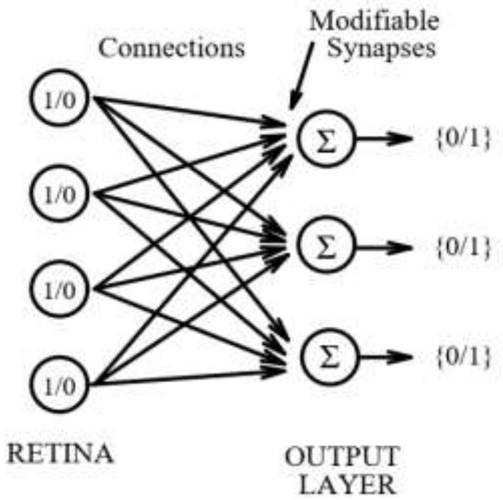


Figure 7. The architecture of a typical perceptron.
Source: [33].

The initial composition of perceptron is two layers of cells connected by synapses that can be modified through learning. The input layer is called the retina. Cells can only assume binary values (for example, 0 or 1) [33].

A model close to the perceptron was the adaline developed by Widrow in 1960.

These early architectures already have most of the essential features of the most modern neural networks. They are composed of simple basic units loosely comparable to neurons. Perceptrons have essentially two layers of cells: an input layer which was called the (artificial) retina of the perceptron, and an output layer. Learning in these networks takes place at the synaptic junctions between the neurons of the input layer and the neurons of the output layer (in the original paper the output layer was called the \association layer"). At first, the performance of these early networks attracted quite a lot of attention. However, their limitations soon became clear [33].

2.6.2 Multilayer Perceptron (Feedforward)

A multilayer perceptron (MLP) known as feedforward neural network, is the main architecture of deep learning. Its objective is to approximate a function f^* [34].

A MLP has three types of layers: input layer, intermediate/hidden layer and output layer and there can be more than one hidden layer. A fundamental property of the MLP is the fact that it is fully connected, which means that every input layer neuron has a connection to every neuron in the hidden layer [34]. The MLP has several neurons structured in layers such input layer, hidden layers and output layers (Figure 8). Output layer with one or many neurons provides output for one or many inputs. In one neuron example, training process task is to find proper weights for neuron connections which in combination with inputs, achieves the desired output.

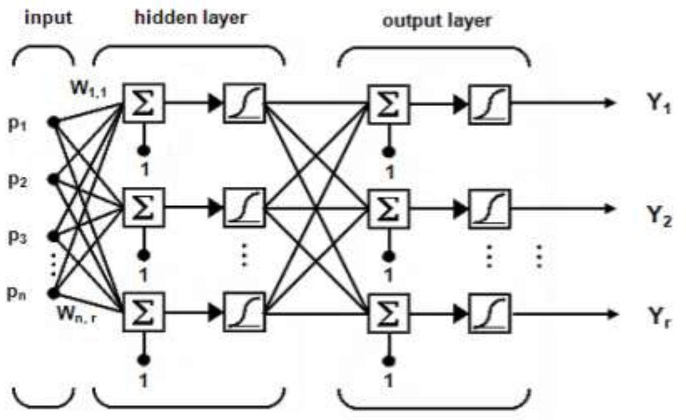


Figure 8. Typical Multilayer Perceptron.
Source: [31].

Feedforward networks can be used for any kind of input to output mapping. A feedforward network with one hidden layer and enough neurons in the hidden layers, can fit any finite input-output mapping problem.

2.6.3 Back Propagation Structure for Network

Back propagation structure propagates the error from the output layer to the hidden layers and changes weights recursively through network from output layer to input layer. The main objective of algorithm is to minimize output error by changing weights. Back propagation algorithm is based on gradient descent. In each step, the goal gradient is computed which direction of negative gradient represents the direction where the surface decreases more rapidly and amount of gradient shows the distance through which the direction is valid [31].

Back propagation also known as cascade feed-forward neural network (CFNN) is a variant of the feedforward network that has additional input connections for each layer and each layer for all subsequent layers [35].

The back propagation method, also known as the error back propagation algorithm, is based on the error-correction learning rule. It consists of two passes through the different layers of the network: a forward pass and a backward pass. In the forward pass, an activity pattern is applied to the input nodes of the network, and its effect propagates through the network layer by layer. Finally, a set of outputs is produced as the actual response of the network [36].

A backpropagation network uses a layered hierarchical architecture of simple neurons (nodes) employing a high degree of connectivity between layers. Only between-layer connections (synapses) are allowed in the ‘simple’ non-recursive networks described here; no within-layer connections may be used. A schematic diagram of a two layered feed-forward network employing full connectivity between adjacent layers is shown in figure 9. It is often overlooked that the backpropagation algorithm does not require complete connection of adjacent layers - restricted connectivity schemes may be employed. Also permitted are synapses which ‘skip’ one or more layers. The only real restriction is that activation can only flow forward in the network, not backward, laterally, or recursively [37].

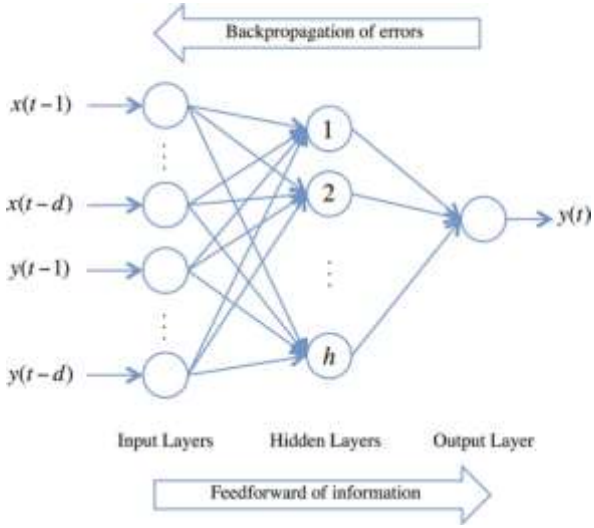


Figure 9. Backpropagation Network Model.
Fonte: [38].

Each node in the network receives one or more inputs from the outside world or from preceding layers, and produces a single output value which is broadcast to other node inputs in succeeding layers. The equations which follow are expressed from the viewpoint of a single node, and should be understood to be carried out over the entire network. The first step in calculating the output of a given node is to determine the net input, which is just the dot product of the node's weight vector with its input vector, given by the Eq. (1) [37].

$$a = \sum_{i=1}^{n} w_i x_i + \theta \tag{1}$$

Where:
x_i represent the inputs to the node;
w_i represent the weights applied to those inputs;
θ is the offset or bias term for the node and;
n is the number of synapses for the node.

Next comes the determination of the node output, which is performed by passing the net input of the node through its transfer function. There are several forms of equations which may be used to implement a sigmoidal transfer function, including the hyperbolic tangent, but the most often used form is shown by the Eq. (2) [37].

$$o = \frac{1.0}{1.0 + e^{-a}} \tag{2}$$

where o is the node output, and a is the net input, from Eq. (1).

For a MLP with n neurons in the input layer, k neuron in a hidden layer and one in the output layer, its mathematical equation can be written as in Eq.(3) [35].

$$y = f^0\left(b_0 + \sum_{j=1}^{k} w_j^0 f_j^h\left(b_j + \sum_{i=i}^{n} w_{ij}^h x_i\right)\right) \tag{3}$$

Where:

f^0 is the activation function of the output layer;

f_j^h is the activation of the hidden layer j;

x_i represents the input;

b_0 is the bias on the output;

b_j is the bias on the hidden layer j and;

y is the output.

A model close to the perceptron was the adaline developed by Widrow in 1960.

3. Materials and Methods

3.1. Data

The database used in this study corresponds to information collected from an industry in the plastic segment of the Manaus Industrial Pole, during the production by injection of PET polymer preforms for the manufacture of carbonated or non-carbonated beverage packaging. Preform will be stored and then delivered to the beverage manufacturer, where it will be produced through the blow molding process of the final packaging for the beverage filling.

Data were collected in the quality control sector in the preforms of 500-piece packaging lots.

An Artificial Neural Network of the Backpropagation type (Cascadeforwardnet) was developed as an intelligent system for prediction of the injection molding process, which is a complex process with a high number of parameters and variables that participate in the process.

The reference for defining the network parameters is based on historical data of the parts produced.

The software used to develop this Intelligent System was MATLAB R2014a® per implementing various types of ANN's through its graphical interface (Toobox) Neural Network Toolbox (NNTool).

The research was defined in two stages, the first characterized by the bibliographic research of computational intelligence applications to industrial processes, and the second occurred with the survey and analysis of the requirements for the control parameters to be used by the proposed ANN.

3.2. Applied Medotology with ANN

The proposed ANN model (figure 8) shows the graphical representation of the MLP of the Cascadeforwardnet type specified for the intelligent ACH prediction system.

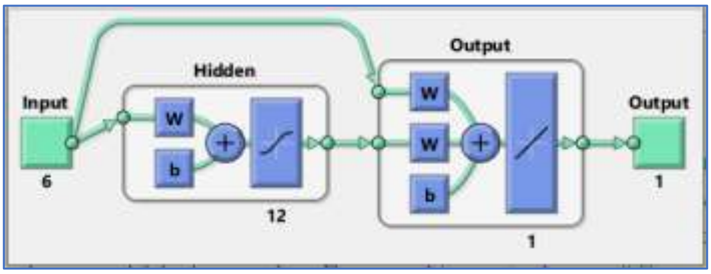


Figure 8. Cascadeforwardnet ANN model for ACH prediction

In figure 1, shows an MLP containing input layer, 1 hidden layer with 12 neurons, 1 output layer with 1 neurons and the network output

The description of the Input/Output parameters used as the basis for the ANN specification, are presented in table 1.

Table 1. Description of Input / Output Parameters.

INPUT	
Dew Point of the grain (D.P)	The lower the air dew point, the faster the drying speed, where the drying air absorption capacity is greater.
	Ranger [10:50].
Residence Time of matter (R.T)	The residence time of the raw material in the silo is, the time that the PET resin stays inside the dryer silo. For PET, it should be four to six hours.
	Ranger [0: 10] hours.
The Initial Humidity of Grains (H.I)	It should not be more than 3,000 *ppm* (0.3%) before its merger. Water absorption by PET resin occurs up to an equilibrium concentration that depends on several factors, such as storage time and temperature, therefore, careful storage in cool and covered environments is recommended.
	Ranger [1000: 6000] *ppm*.
Grain Size (S.G)	The smaller the grain size, the greater the equilibrium moisture in the resin. This effect is attributed to the greater surface area at adsorption (for the same amount of sample, the smaller the grain, the greater the total surface area), this hypothesis is supported by the equilibrium moisture results obtained by PET resin.
	Ranger [0: 10] *mm*.
Grain Temperature (T.G)	Resin in water absorption, resin storage must be maintained at ambient temperatures of 25 ° C, with controlled temperatures in the manufacturing areas.

	Ranger [0: 10] °C.
The Amount of Resin in the Silo (SRA)	The amount of PET resin in the dryer silo must not exceed the consumption that the machine produces in 1 hour continuously.
	Ranger [450:550] kg/h.
OUTPUT	
Temperature Control in the Silo (S.C.T)	Corresponds to the effective temperature of the grains between 160ºC - 180 ° C (measured at the dryer outlet), correct if there is a change in the Acetaldehyde index.
	Ranger [155: 190] °C.

3.2.1 System Parameters

To perform the system controls, the MATLAB R2014a® tool was used and the Neural Network Toolbox (NNTool) was used. In Table 2, the values of the variables used for training and simulation of the Cascadeforwardnet network.

Values of the network simulation variables.

D.P	R.T	H.I	S.G	T.G	S.R.A.	S.C.T
10	3	1000	1	9.5	450	161
45	9	4500	9.0	40	545	161
50	10	5000	10.0	45	550	161
15	4.5	1500	2,5	10	470	162
40	8	4000	8.5	35	540	167
20	4.0	1700	3	15	490	168
35	6	2500	6	25	520	172
25	5.5	2000	4	20	510	173
30	5	3500	5	22.5	500	173
35.5	7	3000	7.5	30	530	173

The set of values of the input variables for training the neural network is shown in figure 9, INPUT matrix:

```
input = [
10.000 45.000 50.000 15.000 40.000 20.000 35.000 25.000 30.000 35.500;
3.0000 9.0000 10.000 4.5000 8.0000 4.0000 6.0000 5.5000 5.0000 7.0000;
1000.0 4500.0 5000.0 1500.0 4000.0 1700.0 2500.0 2000.0 3500.0 3000.0;
1.0000 9.0000 10.000 2.5000 8.5000 3.0000 6.0000 4.0000 5.0000 7.5000;
9.5000 40.000 45.000 10.000 35.000 15.000 25.000 20.000 22.500 30.000;
450.00 545.00 550.00 470.00 540.00 490.00 520.00 510.00 500.00 530.00];
```

Figure 9. ANN's Input data matrix.

The set of values of the output variable/target (Temperature in the Silo), for training the neural network is shown in figure 10, OUTPUT matrix:

```
target = [161 161 161 162 167 168 172 173 173 173];
```

Figure 9: ANN Output data matrix.

Other Cascadeforwardnet network configuration parameters:

- Backpropagation Through Time;
- net.trainFcn = 'traingdx';
- net.trainParam.epochs = 1000;
- net.trainParam.lr = 0.001;
- net.trainParam.time = inf;
- net.layers[1].transferFcn = 'tansig';

4. Results and Discussions

All batches produced have an inspected sample, batches whose Acetaldehyde levels are higher than 4 *ppm* are disapproved and discarded, as specified in the standard by the beverage manufacturer, generating waste of resources. This information is passed on to the responsible technicians, who from then on change the temperature regulation of the polymer drying silo.

Simulations performed by the Cascadeforwardnet network, with the actual input parameter values, provide expert technicians with predictive results of the temperature in the silo (Table 3) supporting the control of the ideal temperature of the silo, during the preform manufacturing process, before the manufacture of the batch of PET's bottles reducing the waste of resources.

Table 3, shows an example of the results of the proposed fuzzy inference model.

Table 3. Values of the network simulation variables.

161	163	161	162	167	168	172	170	173	169

It can be seen in the results presented in table 3, that the output values are within the tolerance margins of the silo temperature for non-generation of Acetaldehyde, allowing to evaluate the adequate values of the input variables that result in the drying process of the resin PET. Allowing better temperature regulation.

By varying the input values, it is possible to evaluate the outputs using the proposed system, obtaining a value that allows support in decision making regarding the silo temperature regulation. In figure 10, the result of the regression test for training the network used.

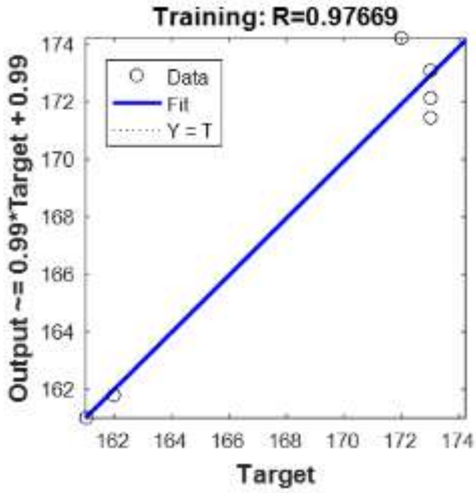


Figure 10. Regression Test, of the Network Training.

The validation of the quality of the network training can be analyzed by regressing aspects of the network training, in which the closer to 1, the better the training, comparing the desired output with that obtained. In figure 11, the result of the regression test of the network validation.

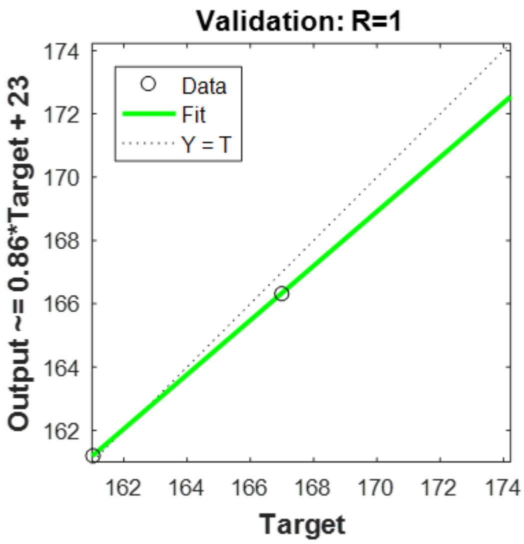


Figure 11. Regression Test, of the Network Validation.

Analyzed by the regression of the validation aspects of the network, it can also be considered that the closer to 1, the better the validation. In figure 12, the results of the regression for the Network test.

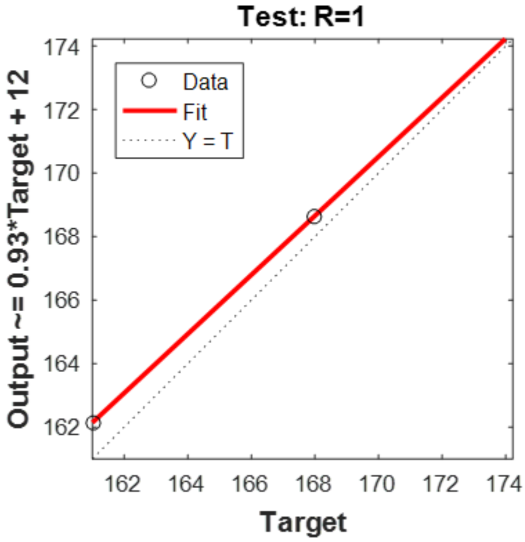


Figure 12. Test Regression, of the Network.

Analyzed by the regression test aspect of the network, it can also be considered that the closer to 1, the better the test. In figure 13, regression for the three aspects in sets of the network.

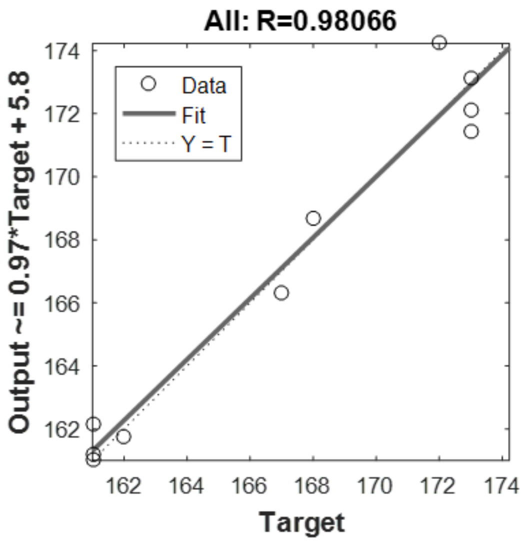


Figure 13. Regression of the joint aspects of the Network.

Another way of validating the quality of the network is the graph that presents the best performance of training validation, which consists of comparing the best result sought, and the behavior of training, validation and testing in the training phase (Figure 14).

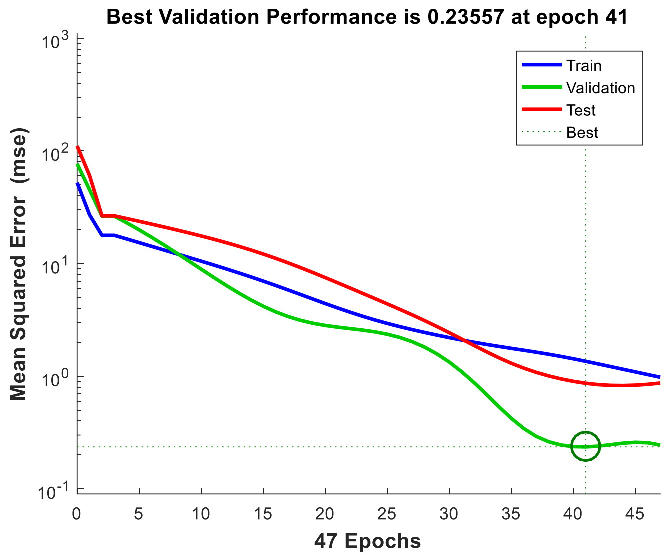


Figure 14. Performance of the Network aspects.

In figure 14, the best training validation performance presented at work can be seen, that is, the values obtained from the training, validation and test achieved with 41 epoch. It is observed that after some attempts to train the network, it was concluded that the validation was close to 0, that is, 0.23557, an expected result given the size of the set of input values for training the network.

5. Conclusion

In this study, an application of Artificial Neural Networks was presented to prevent the generation of Acetaldehyde by controlling the temperature of the drying silo of the PET polymer injection machine. The model was based on input parameters pre-established by the resin manufacturers.

The neural networks of the retro fed type showed results that, in general, from the input information, determine which ideal temperature of the silo so that the production of preforms is with the levels of acetaldehyde within the desired limits for the patterns of quality required by the beverage manufacturer, that is, with Acetaldehyde content below 4ppm. Based on these results, it can be said that the proposed ANN of the Cascadeforwardnet type can be considered as an important tool in controlling the temperature of the silo in the production of PET´s bottles.

For future work, it is suggested the search for an interconnection of the Neuro Fuzzy system with the injector machine controls, so that an automatic control synchronized with the temperature control sensors is carried out, making a fully automated system.

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