APPLICATION OF ARTIFICIAL INTELLIGENCE TECHNIQUES IN THE OPTIMIZATION OF SINGLE SCREW POLYMER EXTRUSION

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Keywords: Data-mining, polymer extrusion, single screw, artificial intelligence, multiobjective optimization

Abstract As with most real optimization problems, polymer processing technologies can be seen as multi-objective optimization problems. Due to the high computation times required by the numerical modelling routines usually available to calculate the values of the objective function, as a function of the decision variables, it is necessary to develop alternative optimization methodologies able to reduce the number of solutions to be evaluated, when compared with the technics normally employed, such as evolutionary algorithms. Therefore, in this work is proposed the use of artificial intelligence based on a data analysis technique designated by DAMICORE surpasses those limitations. An example from single screw polymer extrusion is used to illustrate the efficient use of a methodology proposed.

1. INTRODUCTION

Industrial processes, such as polymer processing, are characterized by a different type of data that can influence decisively its performance. Parameters such as operating conditions, material properties and system geometry have an impact on its functioning since the thermomechanical environment of the process allows obtaining mathematical relations between these design variables and the objectives to be accomplished. Thus, it is possible to optimize directly the process using those routines to evaluate the solutions proposed by the optimization algorithms.

However, are other types of variables that cannot be related directly to the objectives, such for

example, environmental parameters, which can influence the performance of the processes. Also, very often, plenty of experimental data is available that is not used in the optimization.

This work aims to apply Artificial Intelligence techniques to optimize the single screw polymer extrusion process, which is a multi-objective optimization problem consisting in satisfying simultaneously several objectives and constraints. This optimization depends on the definition of the best set of design variables, operating conditions and/or geometrical parameters.

Usually, this problem is solved by associating a numerical modelling routine with optimization algorithms, in which this routine must be run several times, implying necessarily high computation times due to the sophistication of the numerical codes.

An alternative methodology is used to reduce the number of modelling evaluations required during the optimization, which is based on a data analysis technique named DAMICORE, able to define important interrelations between all variables related to extrusion and, then, optimize the process.

The results obtained a practical example agree with the expected thermomechanical behaviour of the process, which demonstrated that AI techniques can be useful in solving practical engineering problems.

This paper is organized as follows: in section 2 important details about the single screw polymer extrusion are introduced, the concepts and the methodology adopted for data-driven optimization are described in section 3, in section 4 the results are presented and discussed, and in section 5 the conclusions are stated.

2. SINGLE SCREW POLYMER EXTRUSION

Polymer extrusion is a technological process where a melted polymer is forced to cross a die at a given output that provides the final shape to the product being made. As can be seen in Figure 1, the extruder machine is constituted by a heated barrel having an Archimedes type screw rotating inside at a prescribed velocity [1-4].

The solid polymer is fed in the hopper and by the action of gravity falls inside the barrel, where, by the action of the screw rotation, is forced to move to the heated barrel zone and, after melting, is pressurized and forced to pass through the die. This process is known as plasticizing and consists of the following steps [1-4]:

- 1) Solids conveying in the hopper: transport of loose pellets in the hopper by the action of gravity;
- 2) Solids conveying in the screw: transport of a solid plug balance resulting from the forces acting in the barrel and screw surfaces due to the friction differences;
- 3) Delay zone: characterized by the development of a melt film near the barrel surface;
- 4) Melting zone: characterized by the development of a specific melting mechanism through the formation of a melt pool near the active screw flank;
- 5) Melt conveying: transport of the melted polymer that results from a balance between the positive flow due to drag and negative flow due to pressure increase;
- 6) Melt pressure flow through the die.

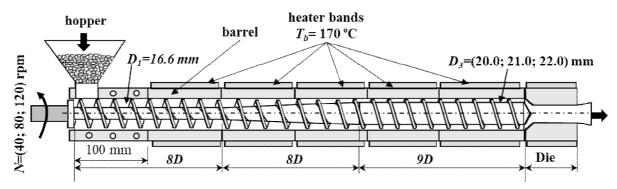


Figure 1. Single screw extruder: geometry and operating conditions.

This is a complex process as is its numerical modelling, which involves the resolution of the differential momentum and energy equations for each one of the stages identified above taking into account, for that purpose, the corresponding boundary conditions and continuity conditions between the stages. Details of this modelling can be found elsewhere [5].

The functioning of the process, as well as its performance, depends on variables related to the properties of the material (physical, thermal and rheological), the geometry of the system (mainly the screw) and the operating conditions (barrel temperature and rotation speed of the screw). Simultaneously, the performance can be measured by taking into account: mass output, melt temperature, length of screw required for melting, mechanical power consumption, mixing degree and viscous dissipation.

Therefore, to optimize the process the decision variables are related to the operating conditions and screw geometry, being the aim to maximize output and mixing and minimize all the other performance measures referred to above [5].

3. DATA-DRIVEN OPTIMIZATION

3.1. Concepts

When dealing with Multi-Objective Optimization Problems (MOOP), it usually requires some interaction with a DM that is the expert in the field. Therefore, the aim here is to use data analysis to reduce these interactions and to provide in the end a very good approximation to the final solution to be used in the real problem studied. This can be done by linking data analysis tools with optimization methodologies to facilitate the search and help the decision-making process, i.e., to use data to drive the optimization.

The use of data-driven optimization can be understood, at least, in two ways:

- the original methodology of calculating the objectives can be replaced by a metamodel or a surrogate model that, making use of available data, can determine the parameters of the model, e.g., polynomial regression [6], kriging [7], Artificial Neural Networks (ANN) [8], radial basis function networks [9], and swarm optimization [10];
- ii) helping the computer to decide on the best solution to use based on existing or

generated data [11].

There are available in the literature different metamodels based on Artificial Intelligence (AI), such as linear and nonlinear regression, incremental dynamic model decomposition [12, 13], Support Vector Machines (SVM) [14], ANNs [15], decision trees, and Code2Vect [16]. Nevertheless, it is necessary to take into account that the possibility of the system being influenced by other variables, not considered when the model is obtained, can constitute a limitation of machine learning.

Based on these characteristics, the aim is to use the DAMICORE (proposed in 2011) framework based on the estimation of distances by compression algorithms, called NCD, to facilitate the investigation in the present scenario where a small amount of data is available and the system can be dependent of external effects [17, 18].

Simultaneously, a Feature Sensitivity Optimisation based on Phylogram Analysis (FS-OPA) will be used to find the set of the principal features of a problem considering a real context, namely in what concerns its feature interactions and their contribution to a target or an objective [17]. The proof of concepts and important experimental results concerning the performance of OPA for difficult combinatorial mono and multi-objective optimization problems can be found elsewhere [18, 19].

DAMICORE method is the core of the FS-OPA mechanisms used to work directly with raw data, i.e., to introduce the process of learning from raw data and to generate models to be used in the optimization.

3.2. DAMICORE and FS-OPA for Data-Driven Optimization

DAMICORE is a builder of models based on phylograms able to deal with any type of data (integer, real and complex numbers, categorical, images, sound, etc., and mixtures of them), and involves the use of three main tasks in sequence:

- 1) The use of the Normalized Compression Distance (NCD) metric to generate a distance matrix from the data [20].
- 2) The use of phylogram based modelling to construct evolutionary trees. DAMICORE uses a distance reconstruction algorithm called Neighbour Joining (NJ) in which the quality of the models is improved by a systematic resampling strategy.
- 3) To perform community detection by analysing the phylograms found previously to extract significant and reliable information from them. For that purpose, a Complex Network approach called Fast Newman (FS) is applied [21]. This is, the aim is to find subgroups of data that share common information (DNA), in the present case designated by clades, which identify the communities.

In practice, data is saved for each object to be analysed, DAMICORE runs NCD to calculate the distance between pairs of data and generates a distance matrix, NJ is applied to this matrix to create a phylogram, and, in the end, FN is running to found the clades (communities).

The application of this methodology to the problem under consideration, single screw extrusion, involves the generation of phylograms with information that can provide two

levels of learning.

In **first-level learning**, the aim is to find clades, each representing a cluster of variables sharing information. For optimization, each one of these clusters represents the set of variables with important interactions. As a result, a table with a list of variables with a cluster per row is obtained.

In **second-level learning**, the FS-OPA calculates the contribution of each clade of variables to the objectives. This is made by measuring the distance between the clades of objectives (oclade) to each variable clade (vclade) using the phylogram obtained. These distances correspond to an estimation of the power of a clade to improve an objective. In some cases, there is the possibility of a clade containing variables and objectives, which need to be separated before the calculation of the distances. In this level, two different matrices are produced, one with the phylogram distances from vclades to oclades and the second with the relative phylograms distances from each variable to each objective.

In the future, this information can be used to implement two additional learning levels, that will not be applied in this work.

Third-level learning, which involves the decomposition of a problem in subgroups having some equivalence and some level of independence, can be used to build a surrogate quantifying the power of a clade to improve an objective. The result of this level will be M Bayesian Networks.

Fourth-level learning, where a multivariate model can be built up from the set of information including the frequency distribution of variable values in each clade, which is the type of model required by an Estimation of Distribution Algorithm [18], a type of evolutionary optimization algorithm. Thus, DAMICORE can produce multivariate probabilistic models that can learn from a small amount of data and help in the optimization process. The result of this level is a multiobjective EDA.

In the present study, the two first levels of learning will be used to study a case using real data, as presented in the next section.

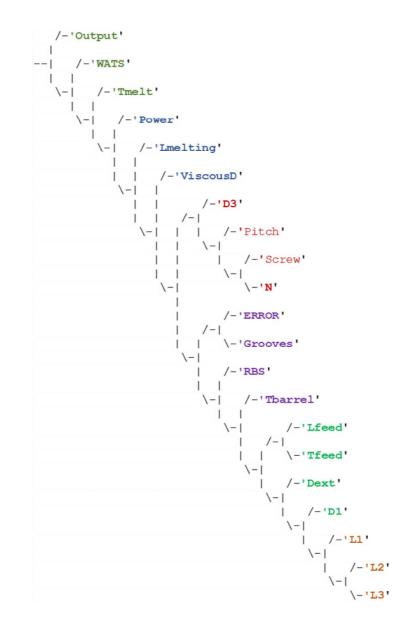
4. RESULTS AND DISCUSSION

4.1. Case Study

As can be seen in Figure. 1, the extruder used has a square pitch screw with a diameter (D) of 25 mm and an L/D ratio equal to 20. It was fitted with a conventional screw with the lengths of the feed, compression, and metering zones equal to 8D, 8D, and 9D, respectively. Different screw geometries were tested, using three internal diameters in the metering zone (D3), i.e., Screw 1 with 22 mm, Screw 2 with 21 mm, and Screw 3 with 20 mm. Screw 2 was also tested for three different pitches (Pitch) in all screw lengths, 20, 25, and 30 mm, respectively.

Concerning operating conditions, the barrel temperature (Tb) was fixed at 170°C, and screw speed was tested for three values, 40, 80, and 120 rpm.

The extruder was used to process a Low-Density Polyethylene, Malen E FGAN 18-D003 from Basell. The viscosity was obtained experimentally using a capillary rheometer the data fitted using the power-law model and the remaining properties were obtained either



from the material manufacturer or the literature.

Figure 2. Single screw extruder: geometry and operating conditions.

Under these conditions, a modelling program based on a numerical method, as referred to in section II above, was used to perform the calculations shown in Table 1. The data was divided into three categories, decision variables, objectives and Error, and is characterized by three types of decision variables: i) data that do not change, e.g., Grooves, RBS, etc.; data that is redundant, e.g., Screw and D3, as they represent the same screw geometry; and data that changes, e.g., Screw, D3, Pitch and N.

The aim is to test the ability of the methodology even in the presence of data that do not have any influence on the objectives. Also, an additional variable is introduced, Error, to take into account the cases that produce results without practical meaning. Only one result is in these conditions.

| Dee | Decision Variables Objectives | | | | | | | | | | Е | | | | | | | | | |
|-----|-------------------------------|-----|------|------|----|-------|-----|-----|-----|-------|-----|-----|-----|--------|-------------------|-------|----------|------|------|---|
| S. | <i>G</i> . | RBS | Dext | D1 | D3 | Lfeed | Ll | L2 | L3 | Pitch | Tf. | Tb | Ν | Output | T _{melt} | Power | Lmelting | WATS | VD | |
| 1 | 0 | 0 | 25 | 16.6 | 22 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 40 | 1.8 | 175.3 | 995 | 6.2 | 315 | 1.04 | 0 |
| 1 | 0 | 0 | 25 | 16.6 | 22 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 80 | 3.5 | 182.1 | 1594 | 12.4 | 296 | 1.36 | 0 |
| 1 | 0 | 0 | 25 | 16.6 | 22 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 120 | 5.2 | 188.6 | 2460 | 13.2 | 299 | 1.25 | 0 |
| 1 | 0 | 0 | 25 | 16.6 | 22 | 100 | 200 | 200 | 225 | 20 | 70 | 170 | 80 | 2.8 | 182.1 | 1953 | 10.6 | 334 | 1.38 | 0 |
| 1 | 0 | 0 | 25 | 16.6 | 22 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 80 | 3.5 | 182.1 | 1594 | 12.4 | 296 | 1.36 | 0 |
| 1 | 0 | 0 | 25 | 16.6 | 22 | 100 | 200 | 200 | 225 | 30 | 70 | 170 | 80 | 4.3 | 182.4 | 1314 | 14.7 | 279 | 1.07 | 0 |
| 1 | 0 | 0 | 25 | 16.6 | 22 | 100 | 200 | 200 | 225 | 20 | 70 | 170 | 40 | 1.7 | 175.1 | 1063 | 6.7 | 319 | 1.19 | 0 |
| 1 | 0 | 0 | 25 | 16.6 | 22 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 40 | 1.8 | 175.3 | 995 | 6.15 | 316 | 1.04 | 0 |
| 1 | 0 | 0 | 25 | 16.6 | 22 | 100 | 200 | 200 | 225 | 30 | 70 | 170 | 40 | 1.8 | 175.4 | 918 | 6.7 | 306 | 1.04 | 0 |
| 1 | 0 | 0 | 25 | 16.6 | 22 | 100 | 200 | 200 | 225 | 20 | 70 | 170 | 120 | 5.1 | 188.1 | 2404 | 14.0 | 329 | 1.39 | 0 |
| 1 | 0 | 0 | 25 | 16.6 | 22 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 120 | 5.2 | 188.6 | 2460 | 13.2 | 299 | 1.25 | 0 |
| 1 | 0 | 0 | 25 | 16.6 | 22 | 100 | 200 | 200 | 225 | 30 | 70 | 170 | 120 | 5.4 | 189.7 | 2224 | 14.7 | 292 | 1.12 | 0 |
| 2 | 0 | 0 | 25 | 16.6 | 21 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 40 | 2.3 | 176.3 | 946 | 8.7 | 263 | 1.04 | 0 |
| 2 | 0 | 0 | 25 | 16.6 | 21 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 80 | 4.6 | 183.2 | 1487 | 15.4 | 245 | 1.08 | 0 |
| 2 | 0 | 0 | 25 | 16.6 | 21 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 120 | 7.1 | 188.8 | 2201 | 17.1 | 219 | 1.11 | 0 |
| 2 | 0 | 0 | 25 | 16.6 | 21 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 40 | 2.1 | 176.1 | 1157 | 6.8 | 295 | 1.04 | 0 |
| 2 | 0 | 0 | 25 | 16.6 | 21 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 40 | 2.3 | 176.3 | 946 | 8.67 | 263 | 1.04 | 0 |
| 2 | 0 | 0 | 25 | 16.6 | 21 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 40 | 2.3 | 176.4 | 966 | 6.8 | 272 | 1.04 | 0 |
| 2 | 0 | 0 | 25 | 16.6 | 21 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 120 | 6.4 | 187.7 | 2425 | 15.7 | 266 | 1.14 | 0 |
| 2 | 0 | 0 | 25 | 16.6 | 21 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 120 | 7.1 | 188.8 | 2201 | 17.1 | 219 | 1.11 | 0 |
| 2 | 0 | 0 | 25 | 16.6 | 21 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 120 | 7.6 | 190.6 | 2116 | 17.6 | 204 | 1.12 | 0 |
| 3 | 0 | 0 | 25 | 16.6 | 20 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 40 | 2.8 | 176.8 | 724 | 14.2 | 210 | 1.04 | 0 |
| 3 | 0 | 0 | 25 | 16.6 | 20 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 80 | 5.9 | 182.9 | 1371 | 17.8 | 157 | 1.08 | 0 |
| 3 | 0 | 0 | 25 | 16.6 | 20 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 120 | 10.2 | 185.2 | 1727 | 21.6 | 70 | 1.09 | 0 |
| 3 | 0 | 0 | 25 | 16.6 | 20 | 100 | 200 | 200 | 225 | 20 | 70 | 170 | 40 | 2.5 | 177 | 1233 | 5.8 | 295 | 1.04 | 0 |
| 3 | 0 | 0 | 25 | 16.6 | 20 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 40 | 2.8 | 176.8 | 724 | 14.2 | 210 | 1.04 | 0 |
| 3 | 0 | 0 | 25 | 16.6 | 20 | 100 | 200 | 200 | 225 | 30 | 70 | 170 | 40 | 2.9 | 177.1 | 668 | 14.9 | 193 | 1.04 | 0 |
| 3 | 0 | 0 | 25 | 16.6 | 20 | 100 | 200 | 200 | 225 | 20 | 70 | 170 | 120 | 7.3 | 185.7 | 2518 | 16.6 | 195 | 1.09 | 0 |
| 3 | 0 | 0 | 25 | 16.6 | 20 | 100 | 200 | 200 | 225 | 25 | 70 | 170 | 120 | 10.2 | 185.2 | 1727 | 21.6 | 70 | 1.09 | 0 |
| 3 | 0 | 0 | 25 | 16.6 | 20 | 100 | 200 | 200 | 225 | 30 | 70 | 170 | 120 | 53.9 | 224.5 | 2432 | 25.0 | 2 | 1.32 | 1 |

Table 1. Data-Set

Before proceeding with the application of the methodology, data is normalized to avoid the comparison between values of different levels. For that, all values in each column were divided by the maximum value found in that column, except in the case the maximum value is zero.

4.2. Global Analysis

First, a global analysis of all data is made. Figure. 2 shows the phylogram obtained. Each

node in this figure corresponds to each column in Table 1, either a variable or an objective. The different colours identify the data that share information, i.e., clusters of information with a small distance between them.

The lower distance between the data shown in this phylogram indicates the sharing of information and mutual influence between variables and/or objectives. The colours in Figure 1 identify the clusters found in the first-level learning. Therefore, two important conclusions can be drawn:

- i) all objectives are strongly interconnected, as they are all located very near;
- ii) variables D3, Pitch, Screw and N, due to their location, are the ones that share more information with the objectives. This is what is expected since the changes in the values of the objectives are produced by changes in these decision variables.

However, it is important to note that some variables may not be related to any useful information for the analysis, such as, for example, to infer how much a decision variable contributes to improving objectives. This apparent interconnection can emerge due to spurious reasons, e.g., an exogenous factor that is not relevant for this analysis. This is the case of Grooves, RBS, Error and Tbarrel since they are near the objectives, but their values do not change. An alternative can be to use additional information that can be obtained from the original data set, e.g., the standard deviation of each column in Table 1. This will not be considered here.

Therefore, accordingly, with these results, D3, Pitch, Screw and N, share information between themselves and the objectives.

Given this information, another way of measuring the potential contribution of a variable to an objective is the normalized average of the distances from the variables to all the objectives, as represented in Table 2, which resulted from the second-level learning. These distances are calculated as the longest path between the oclades and vclades, i.e., the maximum number of edges from all paths in the found phylogram (also called cophenetic distances), which can be calculated using Figure 2.

| Decision Variables | Output | Tmelt | Power | Lmelting | WATS | ViscD | Average |
|-----------------------|--------|-------|-------|----------|------|-------|---------|
| 'D3' | 0.53 | 0.40 | 0.33 | 0.27 | 0.47 | 0.20 | 0.37 |
| 'Grooves' | 0.60 | 0.47 | 0.40 | 0.33 | 0.53 | 0.27 | 0.43 |
| 'RBS' | 0.60 | 0.47 | 0.40 | 0.33 | 0.53 | 0.27 | 0.43 |
| 'Pitch' | 0.60 | 0.47 | 0.40 | 0.33 | 0.53 | 0.27 | 0.43 |
| 'Tbarrel' | 0.67 | 0.53 | 0.47 | 0.40 | 0.60 | 0.33 | 0.50 |
| 'Screw' | 0.67 | 0.53 | 0.47 | 0.40 | 0.60 | 0.33 | 0.50 |
| 'N' | 0.67 | 0.53 | 0.47 | 0.40 | 0.60 | 0.33 | 0.50 |
| 'Lfeed' | 0.80 | 0.67 | 0.60 | 0.53 | 0.73 | 0.47 | 0.63 |
| 'Tfeed' | 0.80 | 0.67 | 0.60 | 0.53 | 0.73 | 0.47 | 0.63 |
| 'Dext' | 0.80 | 0.67 | 0.60 | 0.53 | 0.73 | 0.47 | 0.63 |
| 'D1' | 0.87 | 0.73 | 0.67 | 0.60 | 0.80 | 0.53 | 0.70 |
| 'L1' | 0.93 | 0.80 | 0.73 | 0.67 | 0.87 | 0.60 | 0.77 |
| 'L2' | 1.00 | 0.87 | 0.80 | 0.73 | 0.93 | 0.67 | 0.83 |
| 'L3' | 1.00 | 0.87 | 0.80 | 0.73 | 0.93 | 0.67 | 0.83 |

 Table 2. Results from the second-level learning

From the point of view of the extrusion process, the variables that most influence the objectives are D3 and Pitch, which are two variables related to the geometry of the screw because of the average distance to the objectives (last column of this table) is smaller than for the remaining variables. This is what is expected and is in agreement with the theory, as these variables are recognized by their strong effect in the process, as known by specialists.

4.3. Partial Analysis

To test the influence of the design variables in each one of the objectives, different runs were performed considering only part of the data that improves a specific objective. For that, the data set is ordered by each objective and three studies are made, each one using 100%, 50% and 25% of the better solutions of the data are used in the analysis.

The importance of this study is illustrated in Figure 3, where the trade-off between Output and WATS, both to maximize, is plotted using all values of the data set except the one with variable Error equal to 1. As can be seen, these objectives are in conflict and the solutions are spread in the bi-objectives space and no trend can be observed. Also, it is necessary to take into account that there are other objectives and, thus, is not possible to identify, in this bi-objective space, the non-dominated solutions.

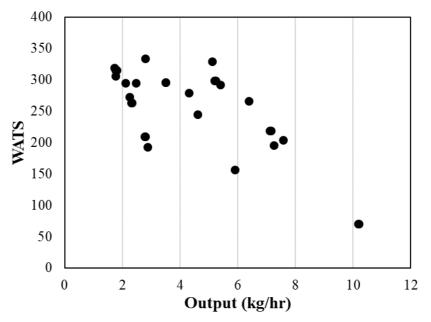


Figure 3. The trade-off between objectives Output and WATS.

Tables 3, 4 and 5 present the same type of results for the second-level learning but know using the 100%, 50% and 25% best solutions, respectively, for output. The order of the distance between the relevant decision variables (i.e., D3, Pitch, Screw and N) changes, which by decreasing order is: for 100% D3, Pitch, Screw, N; for 50% N D3 Screw, Pitch;

and for 25% D3, Screw, Pitch, N. This indicates clearly that for Output the important decision variables are the internal diameter in the metering screw zone (D3) and the screw speed (N), but without a preponderance of one over the other. Again, this is following the knowledge about the process.

| Decision Variables | Output | Tmelt | Power | Lmelting | WATS | ViscD | Average |
|-----------------------|--------|-------|-------|----------|------|-------|---------|
| 'D3' | 0.54 | 0.38 | 0.54 | 0.31 | 0.54 | 0.23 | 0.42 |
| 'RBS' | 0.62 | 0.46 | 0.62 | 0.38 | 0.62 | 0.31 | 0.50 |
| 'Tbarrel' | 0.62 | 0.46 | 0.62 | 0.38 | 0.62 | 0.31 | 0.50 |
| 'Pitch' | 0.62 | 0.46 | 0.62 | 0.38 | 0.62 | 0.31 | 0.50 |
| 'Grooves' | 0.69 | 0.54 | 0.69 | 0.46 | 0.69 | 0.38 | 0.58 |
| 'Screw' | 0.69 | 0.54 | 0.69 | 0.46 | 0.69 | 0.38 | 0.58 |
| 'N' | 0.69 | 0.54 | 0.69 | 0.46 | 0.69 | 0.38 | 0.58 |
| 'Lfeed' | 0.77 | 0.62 | 0.77 | 0.54 | 0.77 | 0.46 | 0.66 |
| 'Tfeed' | 0.77 | 0.62 | 0.77 | 0.54 | 0.77 | 0.46 | 0.66 |
| 'Dext' | 0.77 | 0.62 | 0.77 | 0.54 | 0.77 | 0.46 | 0.66 |
| 'D1' | 0.85 | 0.69 | 0.85 | 0.62 | 0.85 | 0.54 | 0.73 |
| 'L1' | 0.92 | 0.77 | 0.92 | 0.69 | 0.92 | 0.62 | 0.81 |
| 'L3' | 1.00 | 0.85 | 1.00 | 0.77 | 1.00 | 0.69 | 0.89 |
| 'L2' | 1.00 | 0.85 | 1.00 | 0.77 | 1.00 | 0.69 | 0.89 |

Table 3. Results for the 100% better solutions for output

| Decision Variables | Output | Tmelt | Power | Lmelting | WATS | ViscD | Average |
|-----------------------|--------|-------|-------|----------|------|-------|---------|
| 'N' | 0.54 | 0.38 | 0.54 | 0.31 | 0.54 | 0.23 | 0.42 |
| 'RBS' | 0.62 | 0.46 | 0.62 | 0.38 | 0.62 | 0.31 | 0.50 |
| 'Tbarrel' | 0.62 | 0.46 | 0.62 | 0.38 | 0.62 | 0.31 | 0.50 |
| 'D3' | 0.62 | 0.46 | 0.62 | 0.38 | 0.62 | 0.31 | 0.50 |
| 'Grooves' | 0.69 | 0.54 | 0.69 | 0.46 | 0.69 | 0.38 | 0.58 |
| 'Screw' | 0.69 | 0.54 | 0.69 | 0.46 | 0.69 | 0.38 | 0.58 |
| 'Pitch' | 0.69 | 0.54 | 0.69 | 0.46 | 0.69 | 0.38 | 0.58 |
| 'Lfeed' | 0.77 | 0.62 | 0.77 | 0.54 | 0.77 | 0.46 | 0.66 |
| 'Tfeed' | 0.77 | 0.62 | 0.77 | 0.54 | 0.77 | 0.46 | 0.66 |
| 'Dext' | 0.77 | 0.62 | 0.77 | 0.54 | 0.77 | 0.46 | 0.66 |
| 'D1' | 0.85 | 0.69 | 0.85 | 0.62 | 0.85 | 0.54 | 0.73 |
| 'L1' | 0.92 | 0.77 | 0.92 | 0.69 | 0.92 | 0.62 | 0.81 |
| 'L2' | 1.00 | 0.85 | 1.00 | 0.77 | 1.00 | 0.69 | 0.89 |
| 'L3' | 1.00 | 0.85 | 1.00 | 0.77 | 1.00 | 0.69 | 0.89 |

Table 4. Results for the 50% better solutions for output

Finally, Table 6 presents the summary of this analysis for all objectives. The conclusions, taking into consideration the knowledge about the thermomechanical behaviour of the polymer inside the extruder, for the relative importance of the decision variables in the objectives considered individually are the following:

- i) for Output, Lmelting and WATS the most important variables are D3 and N; since there is an alternation between these variables when the percentage of better solutions used in the analysis changes;
- ii) for Tmelt is D3, as in all cases this variable has the lower distance to the objective:

iii) for Power and ViscousD is N because when the solutions with better power consumption are selected (i.e., 50% and 25%) the screw speed has a lower distance to the corresponding objectives.

| Decision Variables | Output | Tmelt | Power | Lmelting | WATS | ViscD | Average |
|-----------------------|--------|-------|-------|----------|------|-------|---------|
| 'D3' | 0.47 | 0.33 | 0.40 | 0.27 | 0.27 | 0.27 | 0.34 |
| 'Screw' | 0.47 | 0.33 | 0.40 | 0.27 | 0.27 | 0.27 | 0.34 |
| 'Pitch' | 0.47 | 0.33 | 0.40 | 0.27 | 0.27 | 0.27 | 0.34 |
| 'Grooves' | 0.60 | 0.47 | 0.53 | 0.40 | 0.40 | 0.40 | 0.47 |
| 'RBS' | 0.60 | 0.47 | 0.53 | 0.40 | 0.40 | 0.40 | 0.47 |
| 'Tbarrel' | 0.73 | 0.60 | 0.67 | 0.53 | 0.53 | 0.53 | 0.60 |
| 'Dext' | 0.73 | 0.60 | 0.67 | 0.53 | 0.53 | 0.53 | 0.60 |
| 'Tfeed' | 0.80 | 0.67 | 0.73 | 0.60 | 0.60 | 0.60 | 0.67 |
| 'Lfeed' | 0.80 | 0.67 | 0.73 | 0.60 | 0.60 | 0.60 | 0.67 |
| 'D1' | 0.80 | 0.67 | 0.73 | 0.60 | 0.60 | 0.60 | 0.67 |
| 'N' | 0.87 | 0.73 | 0.80 | 0.67 | 0.67 | 0.67 | 0.74 |
| 'L1' | 0.93 | 0.80 | 0.87 | 0.73 | 0.73 | 0.73 | 0.80 |
| 'L2' | 1.00 | 0.87 | 0.93 | 0.80 | 0.80 | 0.80 | 0.87 |
| 'L3' | 1.00 | 0.87 | 0.93 | 0.80 | 0.80 | 0.80 | 0.87 |

Table 5. Results for the 25% better solutions for output

This analysis constitutes the first step in the persecution of the next levels of learning, this is, the definition of the order of importance of the decision variables in the objectives to determine a metamodel relating decision variables and objectives that can be used by optimization algorithms.

| Objectives | Percentage | Decision Variables Order | Importance of the decision variables | | |
|------------|------------|--------------------------|--------------------------------------|--|--|
| | 100% | D3, Pitch, Screw, N | | | |
| Output | 50% | N, D3, Screw, Pitch | D3 and N | | |
| | 25% | D3, Screw, Pitch, N | | | |
| | 100% | D3, Pitch, Screw, N | | | |
| Tmelt | 50% | D3, Pitch, N, Screw | D3 | | |
| | 25% | D3, Pitch, Screw, N | | | |
| | 100% | D3, Pitch, Screw, N | | | |
| Power | 50% | N, D3, Screw, Pitch | Ν | | |
| | 25% | N, D3, Screw, Pitch | | | |
| | 100% | D3, Pitch, Screw, N | | | |
| Lmelting | 50% | D3, Pitch, Screw, N | D3 and N | | |
| | 25% | N, D3, Screw, Pitch | | | |
| | 100% | D3, Pitch, Screw, N | | | |
| WATS | 50% | D3, Pitch, Screw, N | D3 and N | | |
| | 25% | Screw, Pitch, N, D3 | 1 | | |
| | 100% | D3, Pitch, Screw, N | | | |
| ViscousD | 50% | D3, Pitch, Screw, N | Ν | | |
| | 25% | N, Pitch, Screw, D3 | | | |

Table 6. Results from the second-level learning

5. CONCLUSIONS

A data mining methodology was applied to a real data set in the field of polymer processing to analyse and optimize a single screw extrusion polymer process. This computational data is characterized by being scarce and was obtained randomly and considered very different aspects of the process, namely, operating conditions, system geometry and optimization objectives.

Two levels of learning based on a methodology designated by DAMICORE were applied to obtain information about the sharing of information between decision variables and objectives and relevant interactions were found, enabling some conclusions about the importance of specific design variables in the objectives.

The results obtained have physical meaning and are following the thermomechanical knowledge about the process.

6. ACKNOWLEDGMENT

This research was partially funded by NAWA-Narodowa Agencja Wymiany Akademickiej, under grant PPN/ULM/2020/1/00125 and European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie Grant Agreement No 734205–H2020-MSCA-RISE-2016. The authors also acknowledge the funding by FEDER funds through the COMPETE 2020 Programme and National Funds through FCT (Portuguese Foundation for Science and Technology) under the projects UID-B/05256/2020, and UID-P/05256/2020, the Center for Mathematical Sciences Applied to Industry (CeMEAI) and the support from the São Paulo Research Foundation (FAPESP grant No 2013/07375-0, the Center for Artificial Intelligence (C4AI-USP), the support from the São Paulo Research Foundation (FAPESP grant No 2019/07665-4) and the IBM Corporation.

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