MULTI-OBJECTIVE OPTIMIZATION OF SINGLE SCREW POLYMER EXTRUSION BASED ON ARTIFICIAL INTELLIGENCE

António Gaspar-Cunha[1*], Francisco Monaco[2], Janusz W. Sikora[3], Alexandre Delbem[4]

[1] IPC-Institute for Polymers and Composites, University of Minho, Guimarães, Portugal; agc@dep.uminho.pt
[2] Institute of Mathematics and Computer Science, University of São Paulo, Brazil; monaco@icmc.usp.br
[3]Lublin University of Technology, 36 Nadbystrzycka Str., 20-618 Lublin, Poland; janusz.sikora@pollub.pl
[4] Institute of Mathematics and Computer Science, University of São Paulo, Brazil; acbd@icmc.usp.br
[*] Correspondence: agc@dep.uminho.pt, University of Minho, Department of Polymer Engineering, Campus de Azurém, Guimarães, Portugal

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Abstract

The performance of the single screw polymer extrusion process depends on the definition of the best set of design variables, including operating conditions and/or geometrical parameters, which can be seen as a multi-objective optimization problem where several objectives and constraints must be satisfied simultaneously. The most efficient way to solve this problem consists in linking a modelling routine with optimization algorithms able to deal with multi-objectives, for example, those based on a population of solutions. This implies that the modelling routine must be run several times, and, thus, the computation time can become expensive, since they are based on the use of sophisticated numerical methods due to the need to obtain reliable results [1]. The aim of this work is to present an alternative based on the use of Artificial Intelligence (AI) techniques in order to reduce the number of modelling evaluations required during the optimization process. This analysis will be based on the use of a data analysis technique, named DAMICORE, able to define important interrelations between all variables related to extrusion and, then, optimize the process [2,3,4]. For that purpose, the results obtained for three practical examples will be presented and discussed. These case studies include the optimization of screw geometrical parameters, barrel grooves section and rotational barrel segment. It will be shown that the results obtained, taking into consideration the design variables, the objectives and the constraints defined, are in agreement with the expected thermomechanical behaviour of the process.

Polymer Extrusion Problem

In a single screw extruder, an Arquimedes type screw rotates inside a heated barrel at a constant speed (N), as illustrated in Figure 1. In this figure are also shown the transversal cuts in the different stages of the process, as indicated by the black arrows representing the thermomechanical phenomena developed inside the barrel [1]: A)) solids conveying of loose pellets in the hopper due to the action of gravity forces; B) solids conveying of a solid plug in the initial turns of the screw due to the balance between the friction forces acting in the barrel and screw root and flights surfaces; C) delay zone, characterized by solids transport where a melt film is formed near the barrel surface due to the heat conducted from the barrel and generated by friction; D) melting zone, where a specific mechanism develops through the formation of a melt pool (B) near the active flank; E) melt conveying, consisting in the flow of melt due to a balance between the positive conveying flow and the negative pressure flow; and F) melt flow through the die.

The mathematical modelling of plasticizing consists of solving the differential momentum and energy equations for each one of the stages identified taking into account the boundary conditions and a continuous link between the different stages [1]. The performance of the machine depends on the polymer properties, operating conditions (screw speed and barrel and die temperature profiles) and screw geometry, and can be quantified by taking into account output, average melt temperature, length of the screw required for melting the polymer, mechanical power consumption, mixing degree and viscous dissipation. This performance is dependent on the system geometry. Figure 1 illustrates the use of a conventional screw, consisting of three zones: feed, compression and metering zones. Within this work, the aim is to study the influence of the use of a Grooved Barrel Section (GBS) in the feed zone and a Rotational Barrel Segment (RBS) in the metering zone, to improve the pressure generated and the mixing induced, respectively. The optimization consists in defining the value of the decision variables, operating conditions and system geometry, that optimize the objectives, i.e., maximization of output and mixing degree, minimization of melt temperature at die exit, mechanical power consumption and the length required to melting [1].

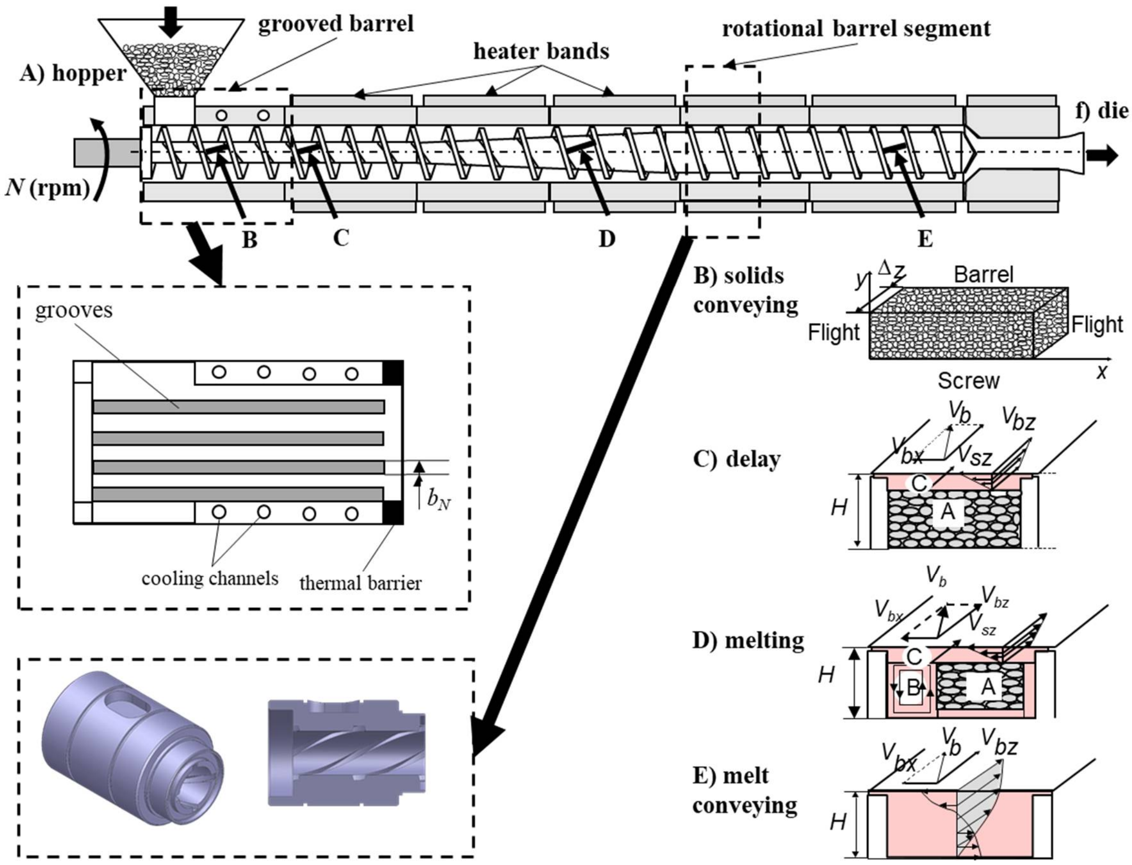

Figure 1- Single screw extrusion: system geometry (barrel, screw, grooved barrel and rotational barrel segment) and plasticizing.

Data-Driven Optimization

The study made here is based on the use of a data analysis technique, named DAMICORE, able to define important interrelations between all variables related to extrusion and, then, optimize the process [2,3,4]. This technique is based in four levels of learning: **First-level learning**. The proposed learning approach finds clades, where each of them is a cluster of variables that share information; while the sharing is relatively poor between clades. For the optimization purpose, each cluster shows a set of variables with significant interactions. **Second-level learning**. The potential contribution of each clade (of the variables in it) to the objectives is evaluated. The output of the second level of learning possesses two matrices: one with the phylogram distances from vclades to oclades and the other with the relative phylogram distances from each variable to each objective. **Third-level learning**. The decomposition of a problem into subgroups (from clades) that has some equivalence, complementarity, a certain level of independence, and their relative power to improve an objective are useful components to compose a surrogate model. **Fourth-level learning**. A multivariate probabilistic model can be constructed from the list of information (in the last above item) together with the frequency distribution of variable values in each clade (or a variation of it). Thus, the output of the fourth level is a multiobjective EDA that can learn from raw data aiming at benefiting the optimization process. In this work, the two first levels of learning are applied to two case studies: a partial and global analysis. In the first case, three different sets will be considered: i) analysis of operating conditions and screw geometry; ii) analysis of grooves section; and iii) analysis of rotational barrel segment. In the latter case, a global analysis with all data is considered.

Figure 9 shows the corresponding phylogram obtained together with other annotations used for levels one and two, in the case of partial analysis of operating conditions and screw geometry. Each leaf node corresponds to a variable (vclade) or an objective (oclade) in the original dataset, where the lines correspond to different solutions/extruder conditions and each column is the values of the decision variables and objectives. This is, each column label in the dataset is the same for its corresponding leaf in the phylogram. The branches in the phylogram with equal colours correspond to leaves of the same clade. Four of them are vclades (dark blue, green, light blue and purple), while the remaining is an oclade (pink). Finally, table 1 shows the normalized average distances from the variables to all objectives resulting from the second-level learning and represents the longest path between oclades and vclades. Thus, in this case, the variables that most influence the objectives are N, Screw, Pitch and D3. This is what is expected, since accordingly to the theory these variables are recognized as having a strong effect on the process.

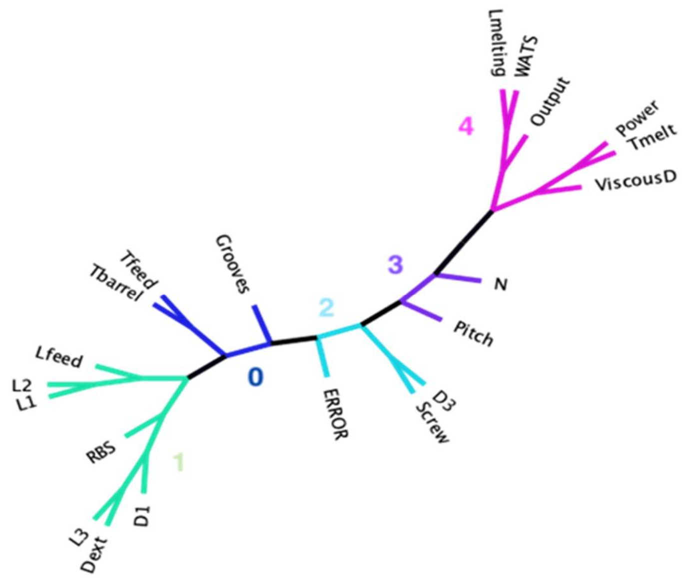

Figure 2- Phylogram obtained by 4LFS-opa from the Screw dataset.

Conclusions

Artificial intelligence technics were applied to analyse and optimize a polymer extrusion process taking into account different process aspects. The computational data used was obtained without taking into consideration any previous process analysis, being similar to random data, and is characterized by being scarce. The main conclusion that can be obtained from this work is that artificial intelligence techniques, based on data-mining, can be used to optimize engineering processes with the use of a few amount of data and without an elaborated problem-oriented optimization strategy. Future work includes the application of the same data at two additional learning levels: third-level learning where the aim will be to obtain a surrogate model relating to the data, which can be used together with an optimization algorithm; and fourth-level learning, which aims to obtain multivariate probabilistic models that can be used as an entire optimization approach.

Table 1- Results from the level-two learning – Screws dataset: relative phylogram distances from each variable to each objective.

	Objectives							
Variables	**Output**	**Tmelt**	**Power**	**Lmelting**	**WATS**	**ViscousD**	**ERROR**	**Average**
N	0.36	0.36	0.28	0.21	0.36	0.36	0.21	0.30
Screw	0.14	0.36	0.36	0.5	0.07	0.28	0.50	0.31
Pitch	0.50	0.50	0.43	0.21	0.50	0.50	0.21	0.40
Grooves	0.43	0.50	0.5	0.50	0.50	0.43	0.21	0.43
D3	0.43	0.50	0.5	0.50	0.50	0.43	0.21	0.43
Tfeed	0.56	0.64	0.64	0.64	0.64	0.56	0.21	0.55
Lfeed	0.71	0.79	0.79	0.79	0.79	0.71	0.36	0.70
Tbarrel	0.71	0.79	0.79	0.79	0.79	0.71	0.36	0.7
L3	0.79	0.86	0.86	0.86	0.86	0.79	0.43	0.77
L2	0.79	0.86	0.86	0.86	0.86	0.79	0.43	0.77
RBS	0.86	0.93	0.93	0.93	0.93	0.86	0.50	0.84
L1	0.86	0.93	0.93	0.93	0.93	0.86	0.50	0.84
D1	0.93	1.00	1.00	1.00	1.00	0.93	0.56	0.91
Dext	0.93	1.00	1.00	1.00	1.00	0.93	0.56	0.91

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