# A REVIEW ON OPTIMIZATION IN POLYMER PROCESSING

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## Abstract

The use of optimization computational tools is of primordial importance for the polymer processing industry, as they provide the means for improving the efficiency of the process without requiring time-consuming and expensive procedures. This review aims to evaluate the application of optimization methodologies to the most important polymer processing technics, including, single and twin-screw extrusion, dies and calibrators, blow-moulding, injection moulding and thermoforming. The most important features of an optimization system will be identified to identify the best practices for each particular situation. These features include the nature of the objective function (single or multi-objective), the type of optimization algorithm, the modelling routine used to evaluate the solutions and the parameters to be optimized. First, the state-of-the-art optimization methodologies generally employed is presented. This will be followed by a detailed review of the literature dealing with this subject. This will be completed by a discussion taking into account the features referred to above. Therefore, it was possible to show that different optimization techniques can be applied to polymer processing with great success.

## Introduction

The processing of thermoplastics encompasses usually three functional steps: melting of a solid polymer, flow and shaping of the melt, and cooling of the final part produced. Thus, to model computationally these processes it is necessary an understanding of heat transfer, melt rheology, fluid mechanics, and morphology development. For that, the modelling routines available are able from input data, such as material properties, system geometry and operating conditions, to calculate performance measures that can help the engineer to select the best solution to use in industrial practice. This can be done using optimization methodologies in such a way that the modelling routine can be run interactively until satisfactory solutions can be found.

Given the importance of understanding optimizing polymer processing techniques a review of literature, applied to single and twin-screw extrusion, dies and calibrators, blow-moulding, injection moulding and thermoforming, is presented. Different alternatives are available in the literature: simulation tools based on a trial-and-error; specific design approaches, i.e., using the modelling equations in a pre-arranged sequence; optimization procedures, in which the process modelling package is used thoughtfully by an optimization algorithm; and perform data-driven optimization, which consists in the use of Artificial Intelligence (AI) techniques to explore the search space based on experimental or computational data.

Given the lack of space, only the analysis concerning the optimization of thermoforming will be presented here.

#### **Application to Polymer Processing**

Figure 1 illustrates the different processing techniques studied in detail by the present review. The methodology used considers the use of the following type of data for thermoforming: i) objective function, that be Single Objective (SO) or Multi-Objective (MO); ii) optimization algorithm, e.g., Empirical, Regression, Direct, Gradient, Simulated Annealing (SA), Evolutionary Algorithm (EA), Inverse Artificial Neural Network (IANN); modelling approach: unidimensional (1D), two-dimensional (2D) and three-dimensional (3D), using Analytical (A), Finite Differences (FD), Finite Volumes (FV) or Finite Elements (FE) approaches; decision variables, i.e., parameters to optimize.



**Figure 1.** Polymer processing sequences are targeted by the review. (A) Single-screw extrusion of profiles (A1), flat film/sheet for thermoforming; (A2), extrusion blow moulding (A3); (B) co-rotating twin-screw compounding and pelletizing (B1); (C) injection moulding: (C1) mould (C2); injection blow moulding. Left: plasticating units; Right: shaping and cooling (with permission from [2] under an open access Creative Common CC BY license).

For each one of the processing techniques identified in Figure 1, a table similar to Table 1 was prepared to compare the methodologies available in the literature using the above type of data [2, 3]. In the present text, only the previous works on optimization for the thermoforming process is presented, as shown in Table 1.

**Table 1.** Previous publications on the optimization of thermoforming (decision variables: OC- operating conditions; TempD- temperature distribution; SThD- sheet thickness distribution) (adapted with permission from [3] under an open access Creative Common CC BY license).

Objective	Optimization	Modelling	Decision	Reference
function	Algorithm	Approach	variables	
SO	Empirical	1D-N	TempD	Duarte and Covas (1997, 2002) [4,5]
SO	Gradient	3D-N	TempD	Wang and Nied (1998) [6]
SO	Gradient	1D-A	TempD	Bordival <i>et al.</i> (2005) [7]
SO	Gradient	3D-N	TempD	Chy and Boulet (2010) [8]
SO	Gradient	3D-N	TempD	Chy et al. (2011) [9]
SO	Regression	3D-N	TempD	Li et al. (2008) [10]
SO	Regression	3D-N	TempD	Li et al. (2010) [11]
SO	SA+EA	3D-N	TempD	Erchiqui et al. (2011 [12])
SO	SA+EA	3D-N	TempD	Bachir-Cherif et al. (2015) [13]
SO	SA+EA	3D-N	TempD	Erchiqui (2018) [14]
SO	Gradient	3D-N	TempD	Bachir-Cherif et al. (2018) [15]
SO	SA+EA	3D-N	TempD	Bachir-Cherif (2019) [16]
SO	IANN	Experimental	OC	Yang and Hung (2004) [17]
SO	IANN	Experimental	OC	Chang et al. (2005) [18]
SO	Regression	Experimental	OC	Leite et al. (2018, 2018) [19,20]
SO	Regression	Experimental	OC	Sasimowski (2018) [21]
MO(2)	EA	3D-N	SThD	Gaspar-Cunha et al. (2021) [22]

## Conclusions

A discussion of the application of optimization methods to solve real problems in single and twin-screw extrusion, dies and calibrators, blow-moulding, injection moulding and thermoforming are presented. Solving these processing challenges as optimization problems is much more efficient than relying on empirical knowledge, or in the use of simulation tools on a trial-and-error basis. Also, can be shown that there is a strong interdependence between the objective function (i.e., the system performance), the optimization algorithm, and data collecting (i.e., experimental or computational data).

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