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A computer based platform to model the intrinsic and final properties of PEAD: application for the injection plastic molding

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Abstract

The continuous development of the advanced computer tools and on-line measurements make possible identifying the reactor operating conditions and relate them to the material properties that are being produced. This is important issue, and specifically for polymers production, in which a broad scenario of applications can be seen. Nowadays, a great challenge related to polymers research has been the development of reliable models enabling prediction of polymer final properties according to the initial operational conditions – either during the polymerization process or from the transformation process phases. The systematic methods, based on modeling and simulation, are fundamental tools to optimize the operational conditions of transformation systems, resulting better products with lower costs. Bearing this in mind, this work aims to built-up empirical models relating some molecular and morphological properties (also knew as intrinsic properties) of polymers and final properties with the reactor operation conditions. A set of statistical tools used in an integrated platform was applied for correlation analysis between all the identified variables and models.

Keywords: Modeling, simulation, correlation, polymer properties

1. Introduction

When producing polymer, the properties must be tailored toward the end use of the product. Moreover, with the enormous competition of polyolefin's market, the knowledge about those properties and their relations with operating conditions become very important for the industry. In fact the polymer supply industries must be able to produce resins with desired final properties in order to satisfy customers.

Plastic injection molding is the primary process for manufacturing plastic parts. Plastic is known to be a very versatile and economical material that is used in many applications. Although the tooling is expensive, the cost per part is very low. Complex geometries are possible and limited only to mold manufacturability, which is affected by the final polymer properties.

Deep knowledge about correlations between final properties and polymer intrinsic properties could be possible way to define the operational conditions of each processing unit in the industry. The fluidity index (FI) and the density are two from the molecular/morphological properties that exert strong influence in the polymer final properties. Thus, the correlations taking into account such properties will be very helpful to define both industrial process units and manufacturing devices to achieve the final product matching customer specifications [1].

2. Problem Statement and background

The product quality is one of the preliminary reasons for using advanced controls in the polymer industry. The material without specification must be sold by reduced price, be mixed with another material, or be wasted. All the three alternatives result in lower profits. However the main problem is to obtain the required set of reactor operational conditions based on feedback information from the desired properties of final use of the polymers. Finally, it is necessary to find out a way to relate the polymeric chain properties or even the final use desired properties with easy to measure operational variables. A possible scheme of the feedback flow of structure polymer information is proposed in Figure 1. This is not easy to be done but important insights can be seen if the final properties of the polymer are expressed as function of the structure properties of the polymeric chains. However, relationships between other molecular/morphological properties (such as spherulite diameter, distance between spherulites) and end-use properties are also necessary. The proposed framework is general and may accommodate all the needed information.

There is a lack of theoretical knowledge regarding how process operation conditions and end-use properties are related [2]. The approach used here to bridge this gap is to identify the relationship between the intrinsic and end-use properties. Also, it is necessary to correlate polymer plant operation conditions with intrinsic properties so that tailor made products may be produced.

According to this strategy, the first step may be regarded to be the most important one, as the second step may be performed with the help of process simulators. Mathematical models are of considerable importance for polymerization engineering, as final polymer properties, and process responses depend upon the process operation conditions in a very complex and non-linear manner [3,4]. Empirical models are a possible workable solution to represent complex systems in which is hard, expensive or too time consuming to develop a detailed to deterministic model. These models try to describe the process behavior, based on experimental evidence.

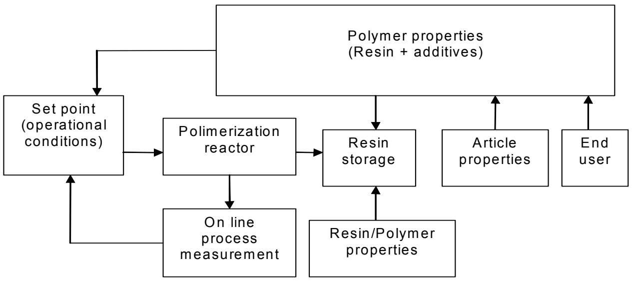

Figure 1 – Simplified scheme on the feedback flow of structure polymer information

3. A Computer Based Platform

The main objective of the present work is built up a workable computer environment based on fundamental tools, including modeling and simulation, for empirical models development relating polymers fundamental and end-use properties. A set of statistical tools used in an integrated platform was utilized for correlation analysis between all the identified variables and models.

3.1. Methodology

In order to carry out the proposed procedure it is necessary to plan a set of experiments for the models development, with the application of each particular polymer final product manufacturing device (for instance, the injection plastic molding). The most important properties to several applications and experiments involving those resins properties were evaluated through from analysis methods, normally used by the resin suppliers. Subsequently, a data treatment was made and empiric models developed, correlating final and intrinsic properties.

Standard correlation analysis was performed for all variables in order to detect the existence of significant correlations. The STATISTICA [5] software was used for this purpose and for model development.

The next step is to relate polymers intrinsic properties with the reactor operating conditions, through the models developed previously. Thus, semi empirical correlations may be useful to model important molecular/morphological properties of polymer (such as the FI, the stress exponent, and polymer density) and process operation variables used routinely to describe the plant operation (such as temperature profiles and head losses in the reaction system).

3.2. Experimental arrangement

A schematic diagram of experimental procedure is showed in Figure 2.

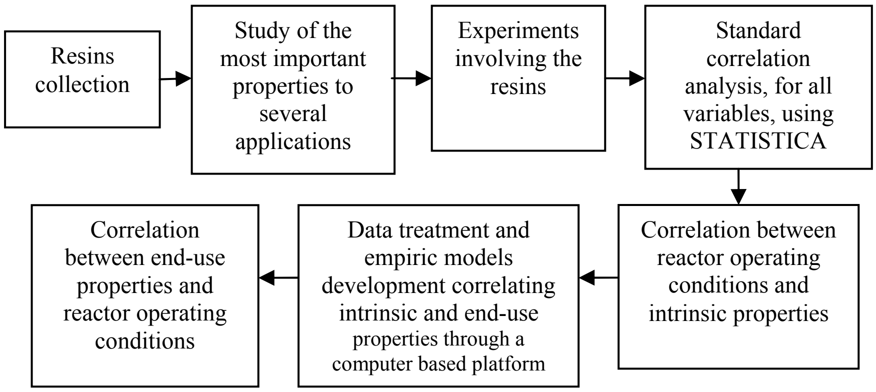

Figure 2 - Schematic diagram of experimental procedure

3.3. Case study

The process studied here is composed of two tubular reactors and a non-ideal stirred tank reactor. The operation is adiabatic and cooling devices are not used. The basic process configuration is shown in Figure 3. Different operation modes may be used in this system, as all reactor vessels are equipped with injection points for all chemical species. Usually, monomer, comonomer, solvent, hydrogen, catalysts, and cocatalysts are fed into the first reactor of the series (which may be reactor #3 or reactor #1), and hydrogen is injected along the reactor train to modify the resin grade. Reactor PFR_{trim} is used as a trimmer, to increase monomer conversion and reduce the amounts of residual light gases at output stream. Besides, the agitators of reactor #1 may be turned off in order to allow the operation of this vessel as a tubular reactor of large diameter. Therefore, depending on the operation mode, the process may be composed of a series of tubular reactors, a continuous stirred tank reactor or some other type of mixed configuration. By changing the operation mode, significant changes of the MWD of the final polymer may be obtained, allowing the production of many resin grades [6].

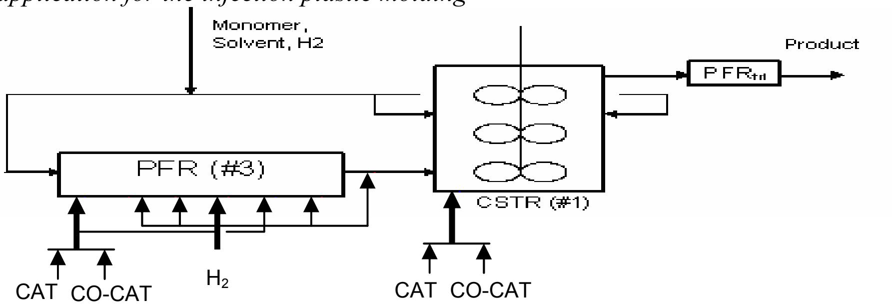

Figure 3 – Basic Process Configuration

After models development that correlates final and intrinsic properties, the next step is to relate polymers intrinsic properties with the reactor operating conditions, through the models encountered previously. Figure 4 illustrates this scheme.

Thirteen linear polyethylene resins for the injection plastic molding were used as specific case study. Eq. (1) and Eq. (2) showed models found for fluidity index (FI) and density. In these models, *Mw* is the polymer molecular weight, *SE* is the polymer stress exponent and CM is the comonomer feed concentration. For the Eq. (1), α= 4,195*1019 (g/10min) and β = -3,9252 (g/10min). For the Eq. (2), α = 0,9424 (g/ml), β = $4{,}08 * 10^{-3}$ (g/ml), γ = $1{,}094 * 10^{-2}$ (g/ml), δ = -56,37 (g/ml), ε = 0,4668 (g/ml).

$$FI = \alpha * Mw^{\beta} \quad (1)$$

$$\rho = \alpha + \beta * \log(FI) + \gamma * SE + \delta * [CM]_e^{\varepsilon} \quad (2)$$

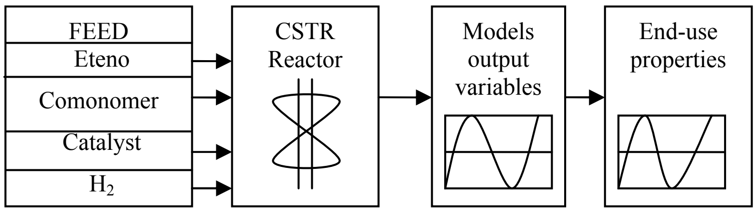

Figure 4 – End-use properties related with reactor output variables.

3.4. Results& discussions

After the models were obtained, an analysis based on errors between the acquired experimental and model calculated values for the end-use properties was made. Figures 5 and 6 show the graphics for the end-use properties. It provides an idea about the models fit to the experimental values.

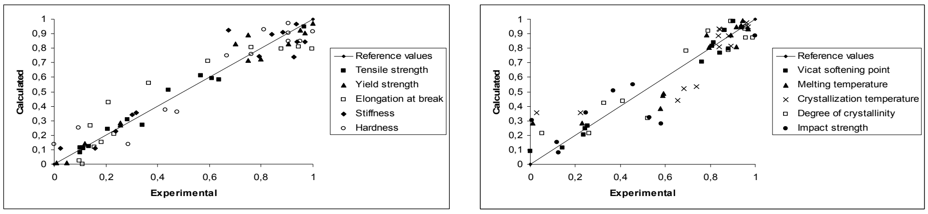

Figure 5 - Comparison between experimental values and calculated values for end-use properties.

4. Conclusions and future work

In this work is proposed a workable computer environment based on fundamental tools, including modeling and simulation and empirical models. It is a suitable environment to help in taking decisions relating process operating conditions with customer specified final products. As a case study, empirical models have been developed to predict end-use properties of polyethylene resins. It may also be concluded that it is possible to model polymer end-use properties as functions of some molecular and morphological properties, such as fluidity index and density in a simple manner, which may have an impact on the company sales strategy of polymer manufacturers. Beyond this, the equations obtained may be used to define process operation in order to obtain a product with desired properties.

Acknowledgements

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