Development of a Virtual Analyzer for Real-Time Monitoring of a Polymer Slurry Process Using Gradient Boosting Algorithms

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Braskem in NUMBERS

INDUSTRIAL UNITS: 41
29 in Brazil, 6 in USA, 4 in Mexico, 2 in Germany

COUNTRIES 100
Exports to clients in some 100 countries

PRODUCTION OF OVER 20 MILLION TONS/YEAR of thermoplastic resins and other chemical products

MORE THAN 7.7k Team Members around the world

EBITDA OF R$ 12.3 BILLION in 2017

NET REVENUE OF R$ 49.3 BILLION in investments in 2017

R$ 167.5 MILLION in innovation investments in 2017

Confidential and/or proprietary information of Braskem
CHEMICALS
MAIN BRANDS & MARKETS
EZOLEM / PLURACT
SENSITIS / UNILENE
POLYOLEFINs

MAIN BRANDS & MARKETS

**INSPiRE:**
- simplified resin management solution

**EVANCE:**
- Sneaker soles

**MAXIO:**
- Fans

**FLEXUS & FLEXUS CLING:**
- Packaging films

**PRISMA:**
- Transparent packaging

**PROEXX:**
- Pet food packaging
- Rice packaging

**RIGEO & RIGEO LUMIOS:**
- Rigid packaging:
  - High-gloss shampoo bottles

**AMPPLEO:**
- Car interiors

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Motivation

- Revolution 4.0: new **Machine Learning** Techniques

- Melt Flow Index (MFI): a measure of the resistance to flow (viscosity) of the polymer melt at a given temperature under a given force for a predetermined period of time (Riley, 2012).

  - Important end-use property (Liu & Yi, 2015).

  - 2 to 4 h for the laboratory analysis to be available (Zhang & Miao, 2015).

- **Soft Sensor**: can provide real-time MFI predictions, allowing a better **process control** and faster decision-making.
Objectives

- **Virtual analyzer** to reduce laboratory demand and off-spec product generation in a large industrial polymer slurry process for production of high-density polyethylene (HDPE).

- Methodology for the choice of time delays between input and output variables of a **gradient boosting regression** (GBR) model, based on statistical analysis and process personnel heuristics.
Figure 1 - Slurry Reaction Unit Flow (Adapted from Mohr, 2004). Summary: 3-Activator Feed, 4-Fresh Hexane Feed, 6-Catalyst Feed, 8-Mother-Liquor Recycle, 9-Ethene Feed, 10-Hydrogen Feed, 11-Suspension Transfer from the First Reactor to the Second Reactor, 12-Comonomer Feed, 13-Reactors 1 Gas Purge, 14-Reactors 2 Gas Purge, 15-Suspension Transfer to the Post-Reactors, 67-Cooling Water Supply, 68-Cooling Water Return.

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Methodology

- Sensor dataset: samples every 1 min.
- Lab MI dataset: samples every 2 or 4 h.
- After joining the two datasets: 7830 samples for training.
Development of a gray-box model for Reactor 1:

- Definition of outliers;
- Merge of grades with similar specifications parameters;
- Selection and treatment of variables (operation ranges, relative importance, correlation, dynamic and static effects, etc.);
- Treatment of intra and inter inconsistencies.
12 input variables:
- temperature
- pression
- hydrogen concentration
- catalyst flow
- level
- hexane flow
- ethene flow
- ethene concentration
- hydrogen flow
- activator flow
- mother-liquor flow
- butene concentration
Gradient Boosting Regressor (GBR)

\[
\{\theta_m, \phi_m\} = \text{argmin}_{\{\theta_m, \phi_m\}} \sum_{i=1}^{n} \left( y_i, f^{(m-1)}(x_i) + \theta_m \phi_m(x_i) \right) \quad (\text{Zemel & Pitassi, 2001})
\]

- \(\phi_m(x)\): simple function
- \(f^{(m-1)}\): current master model
- \(\Theta_m\): weight for the \(m\)th estimator
- \(L_j\): aggregated loss at node

**Figure 2 – Simple Visualization of Gradient Boosting (Adapted from Zhang & Mayer, 2018).**
Delay and window size definition

- Variables division by process dynamics:
  - Group 1: flow measurements
  - Group 2: concentrations
  - Group 3: temperature, level and pressure

- Window definition:
  - Fixed 15 minutes window
  - Decaying ratio: 0.9k, where k is the number of sampling times after the time delay

- Delay selection:
  - GBR regression model smallest RMSE criteria for each group
Delay and window size definition

Delay of Reactor 1:
- Flow: 170 minutes
- Concentration: 130 minutes
- Process (T, L e P): 80 minutes

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## Model Architecture

<table>
<thead>
<tr>
<th>ANN Model</th>
<th>GBR Model</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Hidden Layer</strong></td>
<td><strong>Learning Rate</strong></td>
</tr>
<tr>
<td><strong>Activation Function</strong></td>
<td><strong>Number of estimators</strong></td>
</tr>
<tr>
<td><strong>Iteration</strong></td>
<td><strong>Max depth</strong></td>
</tr>
<tr>
<td>40 neurons</td>
<td><strong>Min samples split</strong></td>
</tr>
</tbody>
</table>

- 80% of the data were used for training and 20% for test.
Results with Linear Regression
Results with Artificial Neural Network
Results with Gradient Boosting Regressor
Model Evaluation

- Root Mean Square Error

\[ \text{RMSE} = \sqrt{\frac{1}{n} \sum_{j=1}^{n} (y_j - \hat{y}_j)^2} \]

- same unit of the model output.
- penalizes the biggest errors.
- but more sensitive to outlier.

<table>
<thead>
<tr>
<th>Model</th>
<th>RMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear Regression</td>
<td>61</td>
</tr>
<tr>
<td>Artificial Neural Network</td>
<td>55</td>
</tr>
<tr>
<td>Gradient Boosting Regressor</td>
<td>49</td>
</tr>
</tbody>
</table>
Conclusions

- A soft sensor was developed for the prediction of MFI of HDPE in an industrial slurry process with the final aim of bringing economical gains by reducing lab demanding and improving process control.

- Expert information integrated with input and output variables correct synchronization in a GBR model drove to successful results.


Thanks!


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