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**Escola Tècnica Superior
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Preparation of a Propane
Dehydrogenation reaction model
for Multi Predictive Control
implementation including
economic optimization

Master thesis presented by Berta Taixés García
to obtain the Master degree in Chemical Engineering
from the Universitat Rovira i Virgili

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Summary

This master thesis report contains all the information about the project *Preparation of a Propane Dehydrogenation reaction model for Multi Predictive Control implementation including economic optimization* performed at the company BASF SONATRACH PropanChem. This document is intended to be evaluated by the members of the jury and includes the description of the student's contribution during the work placement, to be evaluated as well.

The structure of this project is mainly related to the preparation of the MATLAB model for the simulation of the reaction section of the plant, which in this case includes four catalytic reactors and four fired heaters. However, before entering to the main chapters a definition of the scope of the project and a brief description of the plant process is given, followed by the explanation of the student's role in the company during the internship.

Then, there are presented the different sections related to the simulation of the reaction section, to which is first given a more detailed description about the chemistry and operation of the equipment. Later, there are specified, for each equipment, the molar and energy balances and the kinetics and pressure drop models developed as well as the estimations carried out, required for the model. Moreover, the simulation section ends with the presentation of the simulation model and the definition of the specifications required for its functioning.

Afterwards, it is proceeded with the validation of the model, consisting in the simulation of nine pair-of-days of different operating conditions. The results obtained from the latter are then compared to the real plant data, from which is obtained an overall high accuracy and therefore, the MATLAB model has been validated. In addition, there is also included the simulation of the current plant conditions (after the plant's revamping) to provide a good interpretation of the model's outcome.

Furthermore, in order to achieve the main objective of the project it is followed with the optimization of the trials considered, which includes an economic analysis of the main factors affected by the reaction section's behaviour. Besides, to provide a wider scope of the economic analysis mentioned, it is continued with the simulation and later optimization of eight representative trials of the past 4-year run of the plant. From the latter can be given an approximate image of the possibilities provided by the model considering its further implementation in the plant multi predictive control system.

For more information, please contact Pere Gabarra Gironès, General Manager of BASF SONATRACH PropanChem, with email address pere.gabarra-girones@basf.com.