Production of Fuel Grade Ethanol:
Optimization – Based Design, Operation and Control.

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ABSTRACT
The extractive distillation of ethanol using glycerol as entrainer is studied, where a Numerical – Optimization based design, operation and controls were performed. The research includes several steps, where different kinds of numerical optimization are involved. Through the Optimization - based design, it is possible to obtain both optimal operating conditions and optimal design. The solutions of all the optimization problems are achieved using state of the art computational tools and solvers. The results of each stage establishes the process that maximizes an economic criterion for the industrial production of bioethanol satisfying each problem constraints.

Keywords: Fuel Grade Ethanol, Numerical Optimization, Non Linear Programming, Extractive Distillation, Mixed – Integer Non Linear Programming, Biofuels.

1. INTRODUCTION
Biofuels are nowadays viable alternatives to replace fossil fuels worldwide. Biofuels research has been carried out in the past few years thanks to recent interest in renewable energy sources and the benefits of low contamination associated with their use. In several countries, biofuels are produced using traditional chemical processes: for example, in countries like Brazil, Colombia and Thailand, biodiesel is produced from palm oil and alcohol, producing great quantities of glycerol as a byproduct of the process. This overproduction of glycerol has been a source of research for engineers, since an important question emerges: what to do with it?
On the other hand, fuel grade ethanol production implies the need to remove water from it. One way to achieve this is through extractive distillation, an operation that is very energy intensive and that contributes in a considerable way to the total energy requirements of the whole process. In this context, extractive distillation needs an entrainer (a high boiling point compound) in order to achieve the desired ethanol purity, and here is where glycerol comes into play. Using the excess glycerol produced in the biodiesel process it is also possible to produce fuel grade ethanol, as it is shown in figure 1.

This is why the present work is focused in the extractive distillation unit, where a Numerical Optimization – based design, operation and control were performed. It is very important to remark that optimization plays a very important role in the production of biofuels, since it is necessary to produce them in such a manner that makes their prices competitive against fossil fuels [1]. In this context, our research includes several steps, going from the most general case to others more complex. Nevertheless, every step in the research process is essential to achieve the next one.

2. EXTRACTIVE DISTILLATION PROCESS

Extractive distillation is the partial vaporization process that occurs in the presence of a miscible entrainer that alters the relative volatilities of the components present in the mixture to be separated [1]. Adding a new compound to the mixture shifts the thermodynamic equilibrium, modifying the feasible compositions that can be achieved by ordinary distillation. The extractive distillation system is made up by two distillation columns: the first is the extractive distillation column and the second is the entrainer regeneration unit. The flowsheet diagram is shown in figure 2.

3. PRELIMINARY WORK

The stages (past, present and future) included in our research process are addressed next: In the first place, the steady – state (no time - dependence)

![Figure 1. Simplified Flowsheet of the integration between Biodiesel and Bioethanol production.](image-url)
are widely used in the industry and in research due to their apparent simplicity, its mathematical elegance and its predictive capacities [2]. The equations comprised in this model are the following [2]:

- Mass balance: Total and partial for each stage.
- Equilibrium relations: for each component and each stage.
- Mole fraction summations: one for each stage.
- Energy balance: one for each stage.

Here is where the first optimization stage appears, which consists on finding the optimal values of all the column variables in order to minimize annual operating costs. This type of optimization problem is classified as an NLP problem (Non Linear Programming), where there are only algebraic variables, and the model is nonlinear. Up to this point, only preliminary simulations, optimizations and designs were carried out.

4. OPTIMIZATION – BASED DESIGN

In the next stage an optimization – based design was implemented. With the rigorous model tested, we proceed to find (numerically) the optimal column configuration (in terms of design and construction) to minimize the annual operating and capital cost, using an MINLP (Mixed Integer Non Linear Programming) approximation. Results of this stage are very important per se, since its use will allow the extractive distillation column to be built and operated in a real processing facility.

The rigorous design of the extractive distillation system implies establishing the following: areas of the heat exchangers, column diameters, column heights and feed stage locations. It is important to note that these parameters are strictly related to the number of stages of the column. This is why the design variables of the extractive distillation system are the stages in each one of the five column sections: three for the extractive column (rectifying, extractive and stripping) and two for the regeneration column (rectifying and stripping).

The optimization problem of this stage consists of an economic objective function (which consists of discrete and continuous variables) subject to the model constraints (the MESH equations of both columns) and the operational constraints:

\[
\max \ Z = f(x, y) \\
\text{s.t.} \quad h(x) = 0 \\
\quad \quad \quad \quad g(x) \leq 0 \\
\quad \quad \quad \quad x \in X, \ y \in Y
\]  

In Eq. (1) x are the continuous variables, y are the discrete variables, h(x) are the model constraints and g(x) are the operational constraints.
The operational constraints are product requirements in order to meet certain standards for its commercialization:

- Minimum molar purity of ethanol produced: 99.5%.
- Maximum operating temperature allowed in the process (decomposition temperature of glycerol): 555K.

**Objective Function.**

The Objective Function is made up by the following elements:

- Market value of products.
- Raw materials cost.
- Operating Costs: value of the utilities required in the columns operation.
- Infrastructure cost: cost of the columns, additional equipment and installation.

**Solution strategy.**

The solution of the optimization problem is achieved through a two-level strategy. The discrete variables are considered in a master problem that uses a stochastic algorithm in order to evaluate different configurations of the system. The continuous variables are considered in an NLP subproblem that uses a deterministic algorithm in order to find the optimal operating conditions of the system. The implementation of a stochastic algorithm increases the probability of obtaining the global optimum [3]. The model was programmed in Matlab® and was solved on an Intel Core 2 Duo CPU with a 3.07 GHz frequency and 3.21 GB of RAM. The results of this stage are shown in figure 3.

5. **OPTIMAL CONTROL**

However, to achieve steady-state operation in such equipment is a very difficult task. In addition, process variables (e.g. feed flow rate, temperature) can vary as a function of time. Here is where automatic control arises: in response to these variations, the column control system regulates control variables to the point of desired operation of the state variables.

In terms of optimization, an optimal control strategy can be designed to obtain the optimal profiles for a specific time period taking into account the state variables in the extractive distillation column [4]. In this stage, the optimal profile of the control variables (e.g. glycerol feed, energy requirements) that minimizes the operating cost in a determined period of time was obtained, assuming uncertainty (sinusoidal wave) in the feed conditions [5].

It is important to highlight that in this stage it was necessary to change the programming environment to a more specific one, like GAMS (General Algebraic Modelling System). This change was made due to the scale of the model and optimization generated due to the introduction of the time variable (algebro-differential model). This type of problem is classified as a DNLP problem (Dynamic Non Linear Programming), because it has differential and algebraic variables, such as the ones the model has. In this stage, the operational constraints stay the same as the previous stage.

The general formulation of a DNLP problem is as follows:

\[
\min_{x_d(t), x_a(t), u(t), d, \theta(t)} J(x_d(t), x_a(t), u(t), d, \theta(t))
\]  

Subject to:

\[
f(x_d(t), x_a(t), u(t), d) = 0 \quad \forall t \in [t_0, t_f] \\
q(x_d(t), x_a(t), u(t), d) \leq 0 \quad \forall t \in [t_0, t_f] \\
u \in \mathbb{R}^u, \quad d \in \mathbb{D} \\
x_d \in X_d \subseteq \mathbb{R}^{x_d} \\
x_a \in X_a \subseteq \mathbb{R}^{x_a} \\
\theta \in \mathbb{R}^\theta
\]  

In the last equations, \( f \) is the model of the columns and the equations of the control model, and \( q \) are the operative constraints of the process. \( x_d \) are the differential terms of the state variables, \( x_a \) are the differential state variables, \( u \) is the vector of control variables, \( d \) are the design variables and \( \theta \) are the uncertainty parameters. In this case, no design variables are taken into account.
Objective Function.

The objective function of this stage is different from the optimal design in steady state, because it is not an algebraic objective function but an integral objective function over the time variable. It is made up by the following elements:

- Market value of products.
- Raw materials cost.
- Operating costs.

In addition, this objective function has three elements in order to minimize the difference between the steady state operating point and the dynamic operating point. This is made since it is needed to make the transition between two steady states as smooth as possible [6].

Solution strategy.

The algebro–differential model was discretized using finite differences, transforming the DNLP problem into an NLP problem. Because of this, the problem became a sparse large–scale problem. To achieve the solution, an interior point, large scale algorithm available in GAMS was used: IPOPT. This state-of-the-art solver was proven to solve efficiently dense large–scale problems, as well as sparse large–scale problems [7]. The optimization was solved in an Intel i5 CPU with 4 cores, 3.2GHz frequency and 4 GB of RAM. A typical solution of an optimal control problem is shown in figure 4.

6. CURRENT AND FUTURE WORK

The research stages described up to this point are already developed. In the next section the present and future work is described:

It is the intention of the project to combine the optimal design and control in order to accomplish simultaneously these two tasks. The benefits associated with this procedure are that the column can be designed taking into account its controllability and therefore improving its design and operating/capital costs.

If this optimization is accomplished successfully, the column can be far more cost–efficient that the one designed in the MINLP stage. This optimization problem is classified as MIDO (Mixed Integer Dynamic Optimization) in which there are integer, differential and algebraic variables.

Another research that is being conducted intents to compare results of the above extractive distillation column with another case in which external heat sources or sinks are added to the column structure, probably under the MINLP formulation.
7. CONCLUSIONS

The optimization-based research and design proposed considers the elements of design and control with the operation of the extractive distillation for the production of fuel grade ethanol using glycerol as solvent. The approaches reviewed here allow analyzing the feasibility of the process in order to find the most suitable conditions to produce bioethanol. This is achieved through systematic research.

Optimization nowadays, making use of advanced technology and state-of-the-art tools, algorithms and solvers, has become an essential tool in modeling, design and deploy. With optimization techniques one can turn economically infeasible processes into feasible ones. That is why optimization is so important to the industrial sector.

The results obtained in every stage propose a process that offers a very good projection for the industrial production of fuel grade ethanol using glycerol as solvent. As said in the introduction, it is important to produce biofuels in such a way that makes its prices competitive in the market.

8. REFERENCES


